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FILE COVERS 1907 - 15 Jan 2008 VOL 148 ISS 3

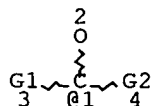
FILE LAST UPDATED: 14 Jan 2008 (20080114/ED)

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<http://www.cas.org/infopolicy.html>

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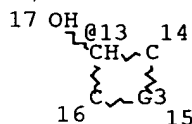
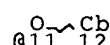
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 L3 287 SEA FILE=CAPLUS ABB=ON PLU=ON DEUTERATION CATALYSTS+PFT,NT/CT  
 L4 2148 SEA FILE=CAPLUS ABB=ON PLU=ON L2 OR L3  
 L5 TRANSFER PLU=ON L4 1- RN : 22168 TERMS  
 L6 22168 SEA FILE=REGISTRY ABB=ON PLU=ON L5  
 L7 952 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (PD OR PT OR RH OR RU OR NI OR CO)/ELS  
 L8 154222 SEA FILE=CAPLUS ABB=ON PLU=ON L7 (L) CAT+NT/RL  
 L10 115 SEA FILE=CAPLUS ABB=ON PLU=ON L2 AND L3 AND L8  
 L11 STR



Ak @5



Cb @8



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REP G3=(0-5) A

VAR G4=1/13

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 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

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L19 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:908108 CAPLUS Full-text

DOCUMENT NUMBER: 147:406255

TITLE: C-H bond activation by water on a palladium or  
 platinum metal surface

AUTHOR(S): Matsubara, Seijiro; Asano, Keisuke; Kajita, Yuichi;  
 Yamamoto, Mitsuru

CORPORATE SOURCE: Department of Material Chemistry, Graduate School of  
 Engineering, Kyoto University, Kyoudai-katsura, Kyoto,  
 606-8501, Japan

SOURCE: Synthesis (2007), (13), 2055-2059  
 CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:406255

AB A water mol. is partially cleaved on a palladium or platinum metal surface  
 under hydrothermal conditions to form an active platinum species. The species  
 is effective for C-H bond functionalization which can be applied for H/D-  
 exchange reactions, C-C bond-forming reactions, and C-N bond-forming  
 reactions.

CC 22-4 (Physical Organic Chemistry)  
 Section cross-reference(s): 66, 67

IT **Deuteration**

**Deuteration catalysts**

(C-H bond activation by water on a palladium or platinum metal surface)

IT **1314-08-5**, Palladium oxide (PdO) **1314-15-4**, Platinum  
 oxide (PtO2) **3375-31-3** **7440-05-3**, Palladium, uses  
**7440-06-4**, Platinum, uses **7440-44-0**, Carbon, uses  
**7718-54-9**, Nickel chloride, uses  
 RL: **CAT (Catalyst use)**; USES (Uses)

(C-H bond activation by water on a palladium or platinum metal surface)

IT 111-67-1P, 2-Octene 112-40-3P, Dodecane 592-98-3P, 3-Octene  
 592-99-4P, 4-Octene 10249-89-5P 20617-93-0P, Quinoxaline-2,3,5,6,7,8-  
 d6 25378-22-7P, Dodecene 32190-42-4P 34071-94-8P, Quinoline-d7  
 36340-20-2P 73509-20-3P, 1H-Indole-1,2,3,4,5,6,7-d7 97797-70-1P  
 97960-58-2P 132125-39-4P 634897-78-2P 688320-42-5P 688320-43-6P  
 688320-44-7P 688320-45-8P 688320-46-9P **688320-48-1P**

880462-22-6P 951164-39-9P 951164-40-2P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(C-H bond activation by water on a palladium or platinum metal surface)

IT **7440-02-0**, Raney nickel, usesRL: **CAT (Catalyst use); USES (Uses)**

(catalysts; C-H bond activation by water on a palladium or platinum metal surface)

IT **1314-08-5**, Palladium oxide (PdO) **1314-15-4**, Platinumoxide (PtO<sub>2</sub>) **3375-31-3 7440-05-3**, Palladium, uses**7440-06-4**, Platinum, uses **7718-54-9**, Nickel chloride, usesRL: **CAT (Catalyst use); USES (Uses)**

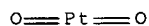
(C-H bond activation by water on a palladium or platinum metal surface)

RN 1314-08-5 CAPLUS

CN Palladium oxide (PdO) (CA INDEX NAME)

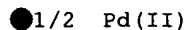
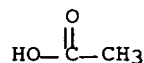


RN 1314-15-4 CAPLUS

CN Platinum oxide (PtO<sub>2</sub>) (CA INDEX NAME)

RN 3375-31-3 CAPLUS

CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)



RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

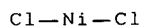


RN 7440-06-4 CAPLUS

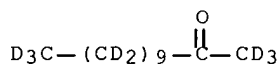
CN Platinum (CA INDEX NAME)



RN 7718-54-9 CAPLUS  
 CN Nickel chloride (NiCl<sub>2</sub>) (CA INDEX NAME)



IT **688320-48-1P**  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (C-H bond activation by water on a palladium or platinum metal surface)  
 RN 688320-48-1 CAPLUS  
 CN 2-Dodecanone-1,1,1,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-d<sub>24</sub>  
 (CA INDEX NAME)



IT **7440-02-0**, Raney nickel, uses  
 RL: **CAT (Catalyst use); USES (Uses)**  
 (catalysts; C-H bond activation by water on a palladium or platinum metal surface)  
 RN 7440-02-0 CAPLUS  
 CN Nickel (CA INDEX NAME)

Ni

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:609303 CAPLUS Full-text  
 DOCUMENT NUMBER: 147:52633  
 TITLE: Process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems  
 INVENTOR(S): Heller, Detleff; Buschmann, Helmut; Drexler, Hans-Joachim  
 PATENT ASSIGNEE(S): Laboratorios Del Dr. Esteve, S.A., Spain  
 SOURCE: Eur. Pat. Appl., 11pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1792887      A1      20070606      EP 2005-384038      20051205
R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
    IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
    BA, HR, MK, YU
WO 2007065891   A1      20070614   WO 2006-EP69313   20061205
W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
    CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
    GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
    KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
    MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
    RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
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    IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
    CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
    GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
    KG, KZ, MD, RU, TJ, TM

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PRIORITY APPLN. INFO.:

EP 2005-384038

A 20051205

OTHER SOURCE(S):

CASREACT 147:52633; MARPAT 147:52633

AB A process for the catalytic hydrogenation/deuteration of C1-6 alkyl ketones, e.g., acetone, (including prochiral ketones) or their deuterated derivs. in high yield and selectivity into their resp. secondary alkanols, e.g., isopropanol, is described. This process comprises using ruthenium achiral or chiral catalytic systems to yield racemic or nonracemic chiral alcs. or deuterated racemic or nonracemic chiral alcs. under high pressure and room temperature

CC 23-8 (Aliphatic Compounds)

Section cross-reference(s): 67

IT **Deuteration****Deuteration catalysts**

Hydrogenation

Hydrogenation catalysts

(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

IT 29841-69-8 **134524-84-8 925941-06-6 939824-57-4**  
**939824-58-5**

RL: **CAT (Catalyst use)**; USES (Uses)

(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

IT **3976-29-2P**, 2-Propan-1,1,1,3,3,3-d6-olRL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

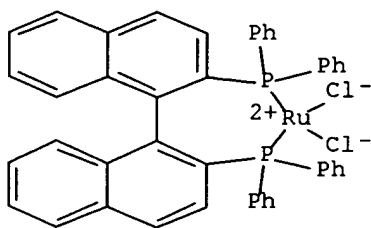
IT **134524-84-8 925941-06-6 939824-57-4**  
**939824-58-5**

RL: **CAT (Catalyst use)**; USES (Uses)

(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

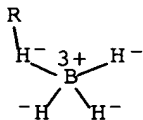
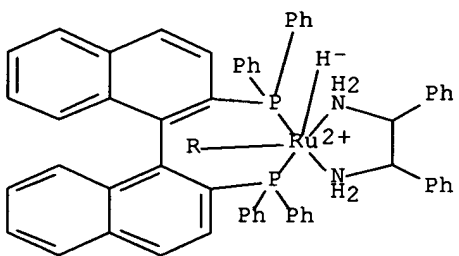
RN 134524-84-8 CAPLUS

CN Ruthenium, [(1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenylphosphine-κP]]dichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



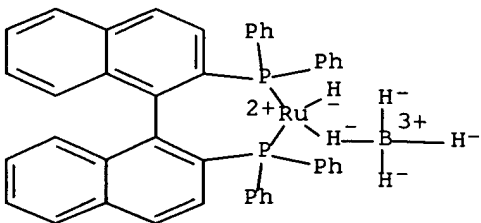
RN 925941-06-6 CAPLUS

CN Ruthenium, [1,1'-(1S)-[1,1'-binaphthalene]-2,2'-diylbis[1,1-diphenylphosphine-κP]] [(1S,2S)-1,2-diphenyl-1,2-ethanediamine-κN1,κN2]hydro[tetrahydroborato(1-)-κH]-, (OC-6-22)- (CA INDEX NAME)



RN 939824-57-4 CAPLUS

CN Ruthenium, [1,1'-(1,1'-binaphthalene)-2,2'-diylbis[1,1-diphenylphosphine-κP]]hydro[tetrahydroborato(1-)-κH]- (CA INDEX NAME)

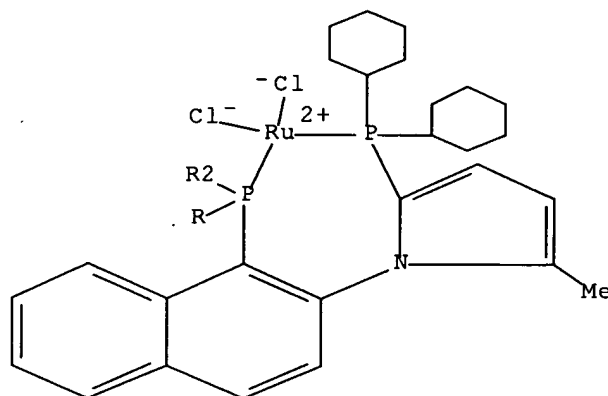


RN 939824-58-5 CAPLUS

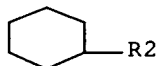
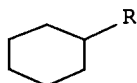
CN Ruthenium, dichloro[2-(dicyclohexylphosphino-κP)-1-[1-(dicyclohexylphosphino-κP)-2-naphthalenyl]-5-methyl-1H-pyrrole]-

(CA INDEX NAME)

PAGE 1-A



PAGE 2-A



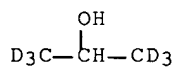
IT 3976-29-2P, 2-Propan-1,1,1,3,3,3-d6-ol

RL: SPN (Synthetic preparation); PREP (Preparation)

(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

RN 3976-29-2 CAPLUS

CN 2-Propan-1,1,1,3,3,3-d6-ol (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1014792 CAPLUS Full-text

DOCUMENT NUMBER: 146:7638

TITLE: C-H/C-D exchange reactions of aromatic compounds in

D2O with NaBD4-activated catalysts  
 AUTHOR(S): Derdau, Volker; Atzrodt, Jens  
 CORPORATE SOURCE: GMPK, Isotope Chemistry & Metabolite Synthesis  
 Frankfurt, Sanofi-Aventis Deutschland GmbH,  
 Frankfurt/Hoechst, 65926, Germany  
 SOURCE: Synlett (2006), (12), 1918-1922  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 146:7638  
 AB A safe and efficient method for catalytic H/D exchange to provide high  
 deuterium incorporation into a variety of aromatic substrates was developed.  
 Systematic screening of the catalyst and activator revealed that the essential  
 activation of the Pd catalyst could be achieved under safe and user friendly  
 conditions. The application of this simple catalytic method for the  
 deuteration of bi- and tricyclic aromatic compds. and chiral natural products  
 was investigated.  
 CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 27  
 IT **Deuteration**  
**Deuteration catalysts**  
 (C-H/C-D exchange reactions of aromatic compds. in D2O with  
 NaBD4-activated catalysts)  
 IT **7440-05-3**, Palladium, uses **7647-10-1**, Palladium(II)  
 chloride  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (C-H/C-D exchange reactions of aromatic compds. in D2O with  
 NaBD4-activated catalysts)  
 IT **37464-79-2P** 651316-73-3P 915232-04-1P 915232-06-3P  
 915232-14-3P 915232-16-5P 915232-18-7P 915232-20-1P 915232-22-3P  
 915232-24-5P 915232-26-7P 915232-28-9P 915232-30-3P 915232-33-6P  
 915232-35-8P  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (C-H/C-D exchange reactions of aromatic compds. in D2O with  
 NaBD4-activated catalysts)  
 IT **7440-05-3**, Palladium, uses **7647-10-1**, Palladium(II)  
 chloride  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (C-H/C-D exchange reactions of aromatic compds. in D2O with  
 NaBD4-activated catalysts)  
 RN 7440-05-3 CAPLUS  
 CN Palladium (CA INDEX NAME)

Pd

RN 7647-10-1 CAPLUS  
 CN Palladium chloride (PdCl2) (CA INDEX NAME)

Cl-Pd-Cl

IT **37464-79-2P**

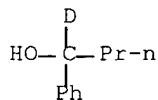


RL: **SPN (Synthetic preparation); PREP (Preparation)**

(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

RN 37464-79-2 CAPLUS

CN Benzenemethan-d-ol,  $\alpha$ -propyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:689620 CAPLUS Full-text

DOCUMENT NUMBER: 146:421688

TITLE: Synergistic effect of a palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reactions of alkyl-substituted aromatic compounds

AUTHOR(S): Ito, Nobuhiro; Watahiki, Tsutomu; Maesawa, Tsuneaki; Maegawa, Tomohiro; Sajiki, Hironao

CORPORATE SOURCE: Chemical Products Research Laboratories, Wako Pure Chemical Industries, Ltd., 1633 Matoba, Kawagoe, 350-1101, Japan

SOURCE: Advanced Synthesis & Catalysis (2006), 348(9), 1025-1028

CODEN: ASCAF7; ISSN: 1615-4150

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A synergistic effect in the H-D exchange reaction of alkyl-substituted aromatic compds. using the Pd/C-Pt/C-D2O-H2 system was discovered. This system would lead to fully H-D exchange results even on the sterically hindered sites which were only low-deuterium incorporated by Pd/C or Pt/C independently. Since the reaction was general for a variety of aromatic compds., it could be applied to the deuteration of dianiline derivs. as raw materials for polyimides.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Deuteration**

**Deuteration catalysts**

Exchange reaction

Exchange reaction catalysts

(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses

RL: **CAT (Catalyst use); USES (Uses)**

(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **767627-97-4P**, Benzene-d5-pentanoic-d8 acid 861405-62-1P

870284-54-1P 870284-60-9P 870284-63-2P 870284-66-5P 870284-69-8P

934266-51-0P 934266-52-1P **934266-54-3P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses

RL: **CAT (Catalyst use); USES (Uses)**

(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

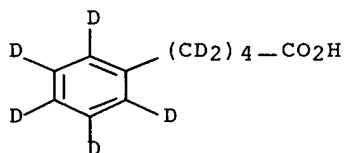
IT **767627-97-4P**, Benzene-d5-pentanoic-d8 acid **934266-54-3P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

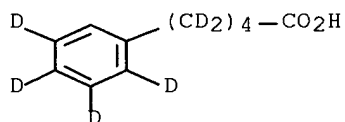
RN 767627-97-4 CAPLUS

CN Benzene-d5-pentanoic-d8 acid (CA INDEX NAME)



RN 934266-54-3 CAPLUS

CN Benzene-2,3,4,5-d4-pentanoic- $\alpha,\alpha,\beta,\beta,\gamma,\gamma$ ,  
 $\delta,\delta$ -d8 acid (CA INDEX NAME)



REFERENCE COUNT:

42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:108991 CAPLUS Full-text

DOCUMENT NUMBER: 144:292970

TITLE: Synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide

AUTHOR(S): Esaki, Hiroyoshi; Aoki, Fumiyo; Maegawa, Tomohiro; Hirota, Kosaku; Sajiki, Hironao

CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Mitahora-higashi, Gifu, 502-8585, Japan

SOURCE: Heterocycles (2005), 66, 361-369

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:292970

AB The D2 gas-free and base-selective H-D exchange reaction of nucleosides was developed. It discloses a convenient route to the post-synthetic incorporation of deuteriums into the base moiety of nucleic acids with high deuterium efficiency.

CC 33-9 (Carbohydrates)

IT **Deuteration**

(regioselective; synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **Deuteration catalysts**

(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **7440-05-3**, Palladium, usesRL: **CAT (Catalyst use)**; USES (Uses)

(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT 24897-52-7P, 2,4(1H,3H)-Pyrimidinedione-5,6-d2 **28671-50-3P**,Cytidine-5-d **40436-51-9P**, Uridine-5-d **40632-21-1P**,Uridine-5,6-d2 **40632-25-5P**, Cytidine-5,6-d2 **74848-84-3P**, Thymidine- $\alpha,\alpha,\alpha$ -d3 **82845-88-3P**,Adenosine-2,8-d2 90742-80-6P **96412-41-8P**, Guanosine-8-d

102147-86-4P 106391-24-6P 200496-79-3P 697807-00-4P,

1H-Purin-2,8-d2-6-amine **697807-01-5P**, Inosine-2,8-d2697807-02-6P **860788-48-3P** **879005-77-3P**,Thymidine- $\alpha$ -d **879005-78-4P**, Thymidine- $\alpha,\alpha$ -d2RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **7440-05-3**, Palladium, usesRL: **CAT (Catalyst use)**; USES (Uses)

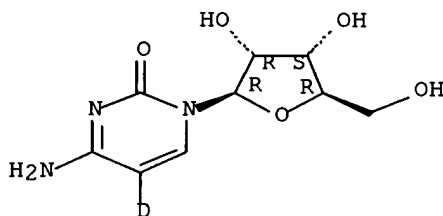
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

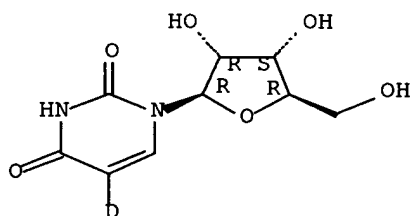
IT 28671-50-3P, Cytidine-5-d 40436-51-9P, Uridine-5-d  
 40632-21-1P, Uridine-5,6-d2 40632-25-5P, Cytidine-5,6-d2  
 74848-84-3P, Thymidine- $\alpha,\alpha,\alpha$ -d3  
 82845-88-3P, Adenosine-2,8-d2 96412-41-8P, Guanosine-8-d  
 697807-01-5P, Inosine-2,8-d2 860788-48-3P  
 879005-77-3P, Thymidine- $\alpha$ -d 879005-78-4P,  
 Thymidine- $\alpha,\alpha$ -d2  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (synthesis of base-selectively deuterium-labeled nucleosides by the  
 pd/C-catalyzed H-D exchange reaction in deuterium oxide)  
 RN 28671-50-3 CAPLUS  
 CN Cytidine-5-d (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



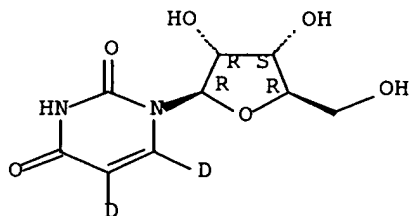
RN 40436-51-9 CAPLUS  
 CN Uridine-5-d (9CI) (CA INDEX NAME)

Absolute stereochemistry.



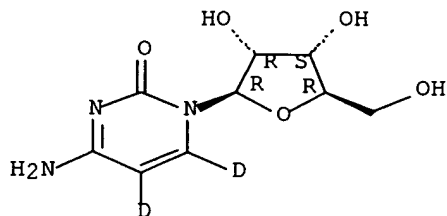
RN 40632-21-1 CAPLUS  
 CN Uridine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



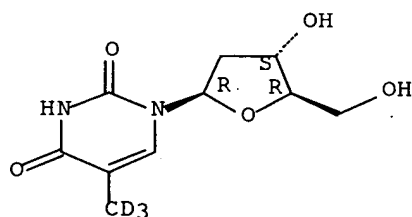
RN 40632-25-5 CAPLUS  
CN Cytidine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



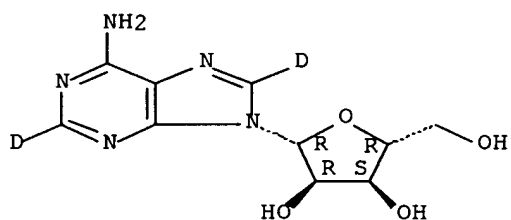
RN 74848-84-3 CAPLUS  
CN Thymidine- $\alpha,\alpha,\alpha$ -d3 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



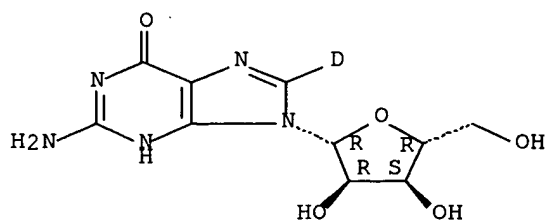
RN 82845-88-3 CAPLUS  
CN Adenosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



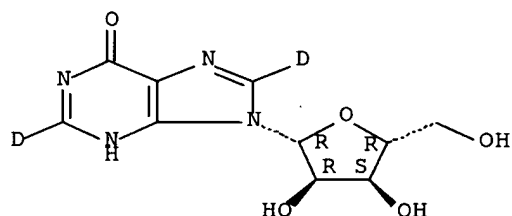
RN 96412-41-8 CAPLUS  
CN Guanosine-8-d (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



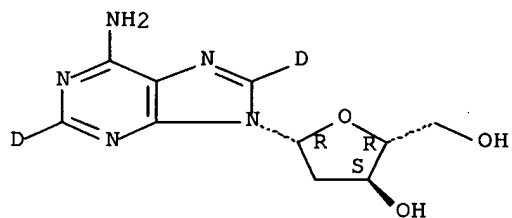
RN 697807-01-5 CAPLUS  
 CN Inosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



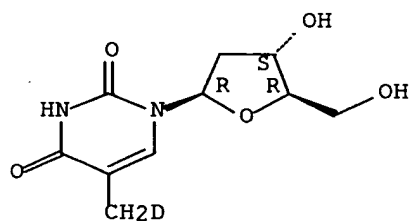
RN 860788-48-3 CAPLUS  
 CN Adenosine-2,8-d2, 2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



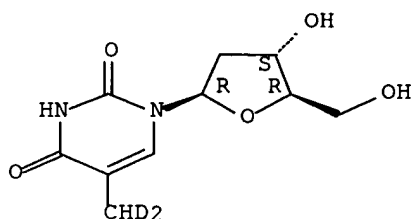
RN 879005-77-3 CAPLUS  
 CN Thymidine-α-d (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 879005-78-4 CAPLUS  
 CN Thymidine- $\alpha,\alpha$ -d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:696848 CAPLUS Full-text  
 DOCUMENT NUMBER: 143:172769  
 TITLE: Method of deuteration of aromatic ring and/or heterocycle compounds using mixed metal catalyst  
 INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao  
 PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070853	A1	20050804	WO 2004-JP19049	20041221
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW:				
BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553376	A1	20050804	CA 2004-2553376	20041221
EP 1707548	A1	20061004	EP 2004-807406	20041221
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1906143	A	20070131	CN 2004-80040874	20041221
PRIORITY APPLN. INFO.:			JP 2004-16075	A 20040123
			WO 2004-JP19049	W 20041221

AB A method of deuteration in which a compound with aromatic ring and/or heterocycle having an enhanced deuteration ratio can be obtained. There is provided a method of deutrating a compound with aromatic ring and/or

heterocycle, characterized in that a compound with aromatic ring and/or heterocycle is reacted with a deuterium source in the presence of an activated mixed catalyst composed of at least two members selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, an iridium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. Thus, 500 mg nicotinic acid, 50 mg Pd/C (5 mg Pd), and 100 mg Pt/C (5 mg Pt) were suspended in 17 mL D<sub>2</sub>O, sealed, purged with H<sub>2</sub>, and heated at 180° for .apprx.24 h to give deuterated nicotinic acid with 99% deuteration at 2, 5, and 6 positions and 48% deuteration at 4 position vs. 98% deuteration at 2 and 5 positions, 99% deuteration at 6 position, and 10% deuteration at 4 position when Pd/C was used alone.

IC ICM C07B059-00

ICS C07C037-00; C07C039-06; C07C051-00; C07C057-30; C07C063-04;  
C07C211-45; C07C209-00; C07D213-803; C07D213-74; C07B061-00;  
C07M005-00

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 25

IT **Deuteration**

**Deuteration catalysts**

(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT **Deuteration**

**Deuteration catalysts**

(regioselective; method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT 7439-88-5, Iridium, uses **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-18-8**, Ruthenium, uses **7440-48-4**, Cobalt, uses

RL: **CAT (Catalyst use)**; USES (Uses)

(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT 1821-12-1P, 4-Phenylbutanoic acid 2438-05-3DP, deuterated derivative 7128-85-0P 7217-47-2DP, deuterated derivative 22527-01-1DP, deuterated derivative 22527-01-1P 66148-15-0P 87385-38-4DP, deuterated derivative **134860-14-3DP**, Benzenebutanoic- $\alpha,\alpha,\beta,\beta,\gamma$  acid, deuterated derivative **358730-86-6P**,

Benzene-d<sub>5</sub>-butanoic-d<sub>6</sub> acid **767627-97-4P**, Benzene-d<sub>5</sub>-pentanoic-d<sub>8</sub> acid **861405-57-4DP**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative **861405-58-5DP**, Benzene-3,4,5-d<sub>3</sub>-pentanoic acid, deuterated derivative **861405-59-6DP**, deuterated derivative **861405-60-9DP**, Benzene-3,4,5-d<sub>3</sub>-butanoic acid, deuterated derivative

861405-61-0DP, deuterated derivative 861405-62-1P 861405-63-2P

861405-64-3DP, deuterated derivative 861405-65-4P 861405-66-5DP,

deuterated derivative 861405-67-6DP, deuterated derivative 861405-68-7P

861405-69-8P 861405-70-1DP, deuterated derivative 861405-71-2P

861405-72-3P 861405-73-4DP, deuterated derivative 861405-74-5DP,

deuterated derivative 861405-75-6P 861405-76-7DP, 3-Pyridine-6-d-

carboxylic acid, deuterated derivative

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-18-8**, Ruthenium, uses **7440-48-4**, Cobalt, uses



RL: **CAT (Catalyst use)**; USES (Uses)

(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS

CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS

CN Ruthenium (CA INDEX NAME)

Ru

RN 7440-48-4 CAPLUS  
 CN Cobalt (CA INDEX NAME)

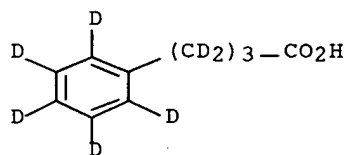
Co

IT **134860-14-3DP**, Benzenebutanoic- $\alpha,\alpha,\beta,\beta,\gamma,\gamma$ -d<sub>6</sub> acid, deuterated derivative **358730-86-6P**, Benzenepentanoic-d<sub>8</sub> acid **767627-97-4P**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative **861405-57-4DP**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative **861405-58-5DP**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative **861405-59-6DP**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative **861405-60-9DP**, Benzenepentanoic-d<sub>8</sub> acid, deuterated derivative  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

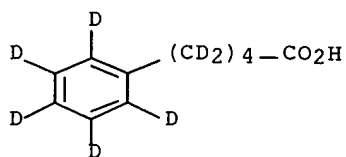
RN 134860-14-3 CAPLUS  
 CN Benzenebutanoic- $\alpha,\alpha,\beta,\beta,\gamma,\gamma$ -d<sub>6</sub> acid  
 (9CI) (CA INDEX NAME)

Ph-(CD<sub>2</sub>)<sub>3</sub>-CO<sub>2</sub>H

RN 358730-86-6 CAPLUS  
 CN Benzene-d<sub>5</sub>-butanoic-d<sub>6</sub> acid (9CI) (CA INDEX NAME)

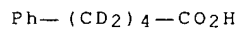


RN 767627-97-4 CAPLUS  
 CN Benzene-d<sub>5</sub>-pentanoic-d<sub>8</sub> acid (CA INDEX NAME)



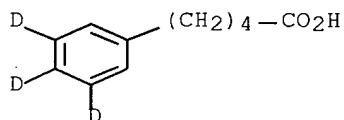
RN 861405-57-4 CAPLUS

CN Benzenepentanoic-d8 acid (9CI) (CA INDEX NAME)



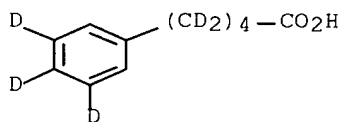
RN 861405-58-5 CAPLUS

CN Benzene-3,4,5-d3-pentanoic acid (9CI) (CA INDEX NAME)



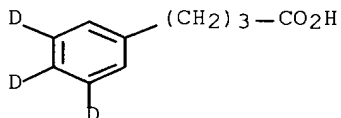
RN 861405-59-6 CAPLUS

CN Benzene-3,4,5-d3-pentanoic- $\alpha,\alpha,\beta,\beta,\gamma,\gamma,\delta$ -d8 acid (9CI) (CA INDEX NAME)



RN 861405-60-9 CAPLUS

CN Benzene-3,4,5-d3-butanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:711257 CAPLUS Full-text

DOCUMENT NUMBER: 141:379678

TITLE: Complete Replacement of H<sub>2</sub> by D<sub>2</sub> via Pd/C-Catalyzed H/D Exchange Reaction

AUTHOR(S): Sajiki, Hironao; Kurita, Takanori; Esaki, Hiroyoshi; Aoki, Fumiyo; Maegawa, Tomohiro; Hirota, Kosaku

CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Gifu, 502-8585, Japan

SOURCE: Organic Letters (2004), 6(20), 3521-3523

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:379678

AB A general and in situ D<sub>2</sub> gas generation method using 10% Pd/C-catalyzed H<sub>2</sub>-D<sub>2</sub> exchange reaction in a H<sub>2</sub>-D<sub>2</sub>O system has been developed. H<sub>2</sub> gas sealed in a reaction flask was efficiently converted into nearly pure D<sub>2</sub> gas, which can be used for the reductive deuteration of substrates possessing reducible functionalities within the mol.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Deuteration**

**Deuteration catalysts**

Hydrogenation

Hydrogenation catalysts

(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

IT **7440-05-3, Palladium, uses**

RL: **CAT (Catalyst use); USES (Uses)**

(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

IT 100-46-9P, Benzylamine, preparation 123-25-1P, Diethyl succinate  
4551-39-7P, 2-Deuteriobenzoic acid 4551-62-6P, 4-Deuteriobenzoic acid

**782486-40-2P, Benzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid-d**

**782486-42-4P, Benzene-3-d-propanoic acid 782486-43-5P,**

Benzene-3-d-ethanol

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

IT **7440-05-3, Palladium, uses**

RL: **CAT (Catalyst use); USES (Uses)**

(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

IT **782486-40-2P, Benzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid-d**

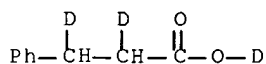
**782486-42-4P, Benzene-3-d-propanoic acid**

RL: **SPN (Synthetic preparation); PREP (Preparation)**

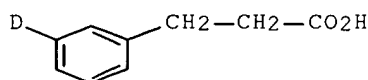
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

RN 782486-40-2 CAPLUS

CN Benzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid-d (9CI) (CA INDEX NAME)



RN 782486-42-4 CAPLUS  
 CN Benzene-3-d-propanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:589514 CAPLUS Full-text  
 DOCUMENT NUMBER: 141:139883  
 TITLE: Method of catalytic deuteration of carbonyl compounds or secondary alcohols by heavy water  
 INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao  
 PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 42 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060831	A1	20040722	WO 2003-JP14182	20031107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2511885	A1	20040722	CA 2003-2511885	20031107
AU 2003277596	A1	20040729	AU 2003-277596	20031107
EP 1577280	A1	20050921	EP 2003-814536	20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1732135	A	20060208	CN 2003-80107483	20031107
US 2006116535	A1	20060601	US 2005-539188	20050616
IN 2005KN01449	A	20070720	IN 2005-KN1449	20050726
PRIORITY APPLN. INFO.:			JP 2002-378932	A 20021227

WO 2003-JP14182 W 20031107

OTHER SOURCE(S): CASREACT 141:139883; MARPAT 141:139883

AB Described is a method of deuterating a carbonyl or secondary alc. compound represented by the general formula R1-X-R2 (I) (wherein R1 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aralkyl ; R2 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aryl, aralkyl, alkoxy, aryloxy, hydroxy; X carbonyl, hydroxymethylene), which comprises reacting the compound represented by the general formula I with a deuterium source, in particular D2O, in the presence of a catalyst selected among activated palladium, platinum, rhodium, ruthenium, nickel, and cobalt catalysts. By the method, deuteration, which has been conducted under severe conditions, can be conducted under neutral conditions. Even when the compound contains an unsatd. bond, it can be deuterated without reducing the unsatd. bond. Not only hydrogens near the carbonyl or hydroxymethylene group but also those remotely situated from these groups are selectively deuterated without deuterating the carbon-carbon double or triple bonds. Thus, 500 mg tricyclo[5.2.1.0<sup>2</sup>'6]decan-8-ol and 100 mg Pd-C were suspended in 17 mL D2O, purged with H<sub>2</sub>, and heated at 180° for 24 h in an oil bath to give tricyclo[5.2.1.0<sup>2</sup>'6]decan-8-ol deuterated by 96% at 8-position and 88% at other positions.

IC ICM C07B059-00

ICS C07C029-00; C07C031-02; C07C035-08; C07C035-29; C07C035-37;  
C07C045-00; C07C049-04; C07C049-08; C07C049-433; C07C049-453;  
C07C051-00; C07C053-10; C07C053-124; C07C057-04; C07M005-00

CC 21-2 (General Organic Chemistry)

IT **Deuteration****Deuteration catalysts**

(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **7440-02-0**, Raney nickel, usesRL: **CAT (Catalyst use)**; USES (Uses)

(catalysts; catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-16-6D**, Rhodium, supported on alumina **7440-16-6D**, Rhodium, supported on carbon **7440-18-8**, Ruthenium, uses **7440-18-8D**, Ruthenium, supported on carbon **7440-48-4**, Cobalt, uses

RL: **CAT (Catalyst use)**; USES (Uses)

(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 79-31-2DP, Isobutyric acid, deuterated 108-93-0DP, Cyclohexanol, deuterated **666-52-4P**, 2-Propanone-1,1,1,3,3,3-d<sub>6</sub> 13380-89-7DP, Tricyclo[5.2.1.0<sup>2</sup>'6]decan-8-ol, deuterated **14044-94-1P** 18153-61-2DP, Bicyclo[2.2.1]heptan-2-one-3,3-d<sub>2</sub>, deuterated **21273-02-9DP**, Cyclohexan-1-d-ol, deuterated 51209-49-5P, Cyclohexanone-d<sub>10</sub> **53481-06-4P** **55935-44-9P** 63870-91-7DP, Norbornenol, deuterated **64118-21-4P** **91468-78-9DP**, Bicyclo[2.2.1]heptan-2-d-2-ol, deuterated **350820-09-6P** **725242-18-2P**, 4-Heptanone-d<sub>14</sub> 725242-19-3DP, deuterated 725242-21-7DP, deuterated **725242-22-8P**, 2-Heptanone-d<sub>14</sub> **725242-23-9P**, 3-Heptanone-d<sub>14</sub> **725242-24-0P**, 2-Heptanol-d<sub>15</sub> **725242-25-1P**, 4-Heptanol-d<sub>15</sub> **725242-26-2DP**, deuterated **725242-27-3DP**, deuterated **725242-28-4DP**, deuterated **725242-29-5DP**, deuterated **725242-29-5P** **725242-30-8P**

725242-31-9P 725242-32-ODP, deuterated

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(catalytic deuteration of carbonyl compds. or secondary alc. compds.  
with heavy water in presence of palladium, platinum, rhodium,  
ruthenium, or nickel)

IT 7440-02-0, Raney nickel, uses

RL: **CAT (Catalyst use); USES (Uses)**

(catalysts; catalytic deuteration of carbonyl compds. or secondary alc.  
compds. with heavy water in presence of palladium, platinum, rhodium,  
ruthenium, or nickel)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

IT 7440-05-3, Palladium, uses 7440-05-3D, Palladium,  
supported on carbon 7440-06-4, Platinum, uses 7440-06-4D  
, Platinum, supported on carbon 7440-16-6, Rhodium, uses  
7440-16-6D, Rhodium, supported on alumina 7440-18-8,  
Ruthenium, uses 7440-18-8D, Ruthenium, supported on carbon  
7440-48-4, Cobalt, uses

RL: **CAT (Catalyst use); USES (Uses)**

(catalytic deuteration of carbonyl compds. or secondary alc. compds.  
with heavy water in presence of palladium, platinum, rhodium,  
ruthenium, or nickel)

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS  
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-16-6 CAPLUS  
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS  
CN Ruthenium (CA INDEX NAME)

Ru

RN 7440-18-8 CAPLUS  
CN Ruthenium (CA INDEX NAME)

Ru

RN 7440-48-4 CAPLUS  
CN Cobalt (CA INDEX NAME)

Co

IT **666-52-4P**, 2-Propanone-1,1,1,3,3,3-d6 **14044-94-1P**  
**21273-02-9DP**, Cyclohexan-1-d-ol, deuterated **53481-06-4P**  
**55935-44-9P** **64118-21-4P** **91468-78-9DP**,  
Bicyclo[2.2.1]heptan-2-d-2-ol, deuterated **350820-09-6P**  
**725242-18-2P**, 4-Heptanone-d14 **725242-22-8P**,  
2-Heptanone-d14 **725242-23-9P**, 3-Heptanone-d14  
**725242-24-0P**, 2-Heptanol-d15 **725242-25-1P**,  
4-Heptanol-d15 **725242-26-2DP**, deuterated **725242-27-3DP**



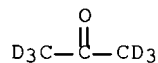
, deuterated 725242-28-4DP, deuterated 725242-29-5DP,  
deuterated 725242-29-5P 725242-30-8P  
725242-31-9P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(catalytic deuteration of carbonyl compds. or secondary alc. compds.  
with heavy water in presence of palladium, platinum, rhodium,  
ruthenium, or nickel)

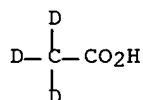
RN 666-52-4 CAPLUS

CN 2-Propanone-1,1,1,3,3,3-d6 (9CI) (CA INDEX NAME)



RN 14044-94-1 CAPLUS

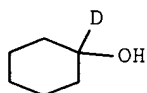
CN Acetic-d3 acid, sodium salt (8CI, 9CI) (CA INDEX NAME)



● Na

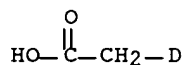
RN 21273-02-9 CAPLUS

CN Cyclohexan-1-d-ol (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 53481-06-4 CAPLUS

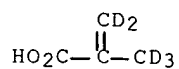
CN Acetic-d acid, sodium salt (9CI) (CA INDEX NAME)



● Na

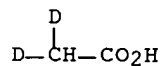
RN 55935-44-9 CAPLUS

CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)- (CA INDEX NAME)



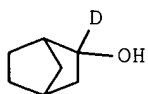
RN 64118-21-4 CAPLUS

CN Acetic-d2 acid, sodium salt (9CI) (CA INDEX NAME)



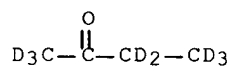
RN 91468-78-9 CAPLUS

CN Bicyclo[2.2.1]heptan-2-d-2-ol (9CI) (CA INDEX NAME)



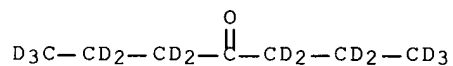
RN 350820-09-6 CAPLUS

CN 2-Butanone-1,1,1,3,3,4,4,4-d8 (9CI) (CA INDEX NAME)



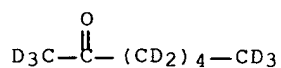
RN 725242-18-2 CAPLUS

CN 4-Heptanone-1,1,1,2,2,3,3,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



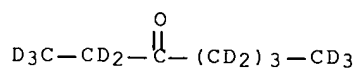
RN 725242-22-8 CAPLUS

CN 2-Heptanone-1,1,1,3,3,4,4,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



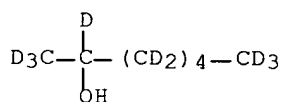
RN 725242-23-9 CAPLUS

CN 3-Heptanone-1,1,1,2,2,4,4,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



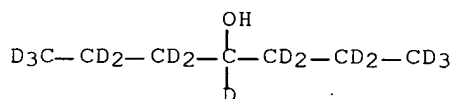
RN 725242-24-0 CAPLUS

CN 2-Heptan-1,1,1,2,3,3,4,4,5,5,6,6,7,7,7-d15-ol (9CI) (CA INDEX NAME)



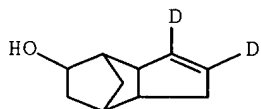
RN 725242-25-1 CAPLUS

CN 4-Heptan-1,1,1,2,2,3,3,4,5,5,6,6,7,7,7-d15-ol (9CI) (CA INDEX NAME)



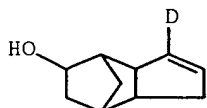
RN 725242-26-2 CAPLUS

CN 4,7-Methano-1H-inden-2,3-d2-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)

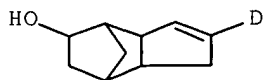


RN 725242-27-3 CAPLUS

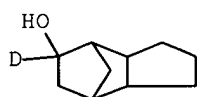
CN 4,7-Methano-1H-inden-3-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



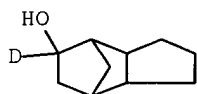
RN 725242-28-4 CAPLUS  
 CN 4,7-Methano-1H-inden-2-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



RN 725242-29-5 CAPLUS  
 CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



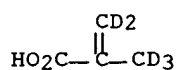
RN 725242-29-5 CAPLUS  
 CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-30-8 CAPLUS  
 CN 4,7-Methano-1H-inden-1,1,2,3,6,7,7-d7-5-ol, octahydro-2,3,3a,4,5,6,7,7a-d8- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 725242-31-9 CAPLUS  
 CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)-, sodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:453150 CAPLUS Full-text  
 DOCUMENT NUMBER: 141:23545  
 TITLE: Method for deuteration or tritiation of heterocyclic compounds  
 INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao  
 PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 45 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046066	A1	20040603	WO 2003-JP14181	20031107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2506010	A1	20040603	CA 2003-2506010	20031107
AU 2003277595	A1	20040615	AU 2003-277595	20031107
EP 1561741	A1	20050810	EP 2003-811499	20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1714060	A	20051228	CN 2003-80103924	20031107
US 2006025596	A1	20060202	US 2005-534344	20050509
IN 2005KN01145	A	20061110	IN 2005-KN1145	20050615
PRIORITY APPLN. INFO.:			JP 2002-331594	A 20021115
			WO 2003-JP14181	W 20031107
AB	A method for deuteration or tritiation of a heterocyclic ring comprises allowing a heterocyclic compound to be present under a sealing and refluxing condition in a deuterated or tritiated solvent (e.g., D2O) in the presence of an activated catalyst selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. The method allows a deuteration or tritiation temperature to be kept at a temperature higher than the boiling temperature of the solvent, which results in the replacement of a hydrogen atom in a heterocyclic ring of a heterocyclic compound with very good efficiency. Further, the method can be widely used for the deuteration or tritiation of various types of heterocyclic compds. in a com. process.			
IC	ICM C07B059-00 ICS C07D209-08; C07D209-20; C07D213-06; C07D231-12; C07D233-58; C07D235-08; C07D239-47; C07D239-54; C07D471-04; C07D473-30; C07D473-34; C07H019-067; C07H019-167; C07M005-00			
CC	28-16 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 26, 33, 34			
IT	<b>Deuteration</b> Tritiation (method for deuteration or tritiation of heterocyclic compds.)			
IT	<b>Deuteration catalysts</b> Tritiation catalysts (palladium and platinum, in method for deuteration or tritiation of			

heterocyclic compds.)

IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses  
7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses  
7440-18-8, Ruthenium, uses 7440-44-0, Carbon, uses  
7440-48-4, Cobalt, uses

RL: CAT (Catalyst use); USES (Uses)

(method for deuteration or tritiation of heterocyclic compds.)

IT 4166-68-1P 6745-43-3P, 1H-Imidazole-2,4,5-d3 22194-79-2P  
24897-52-7P, 2,4(1H,3H)-Pyrimidinedione-5,6-d2 40632-21-1P,  
Uridine-5,6-d2 62595-11-3P, L-Tryptophan-2,4,5,6,7-d5  
82845-88-3P, Adenosine-2,8-d2 96412-41-8P, Guanosine-8-d  
106391-24-6P 130317-91-8P 200496-79-3P 350818-65-4P 697806-98-7P  
697806-99-8P 697807-00-4P, 1H-Purin-2,8-d2-6-amine 697807-01-5P  
, Inosine-2,8-d2 697807-02-6P 697807-03-7P 697807-04-8P  
697807-05-9P 697807-06-0P 697807-07-1P

RL: IMF (Industrial manufacture); SPN (Synthetic  
preparation); PREP (Preparation)

(method for deuteration or tritiation of heterocyclic compds.)

IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses  
7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses  
7440-18-8, Ruthenium, uses 7440-48-4, Cobalt, uses

RL: CAT (Catalyst use); USES (Uses)

(method for deuteration or tritiation of heterocyclic compds.)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS

CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS  
 CN Ruthenium (CA INDEX NAME)

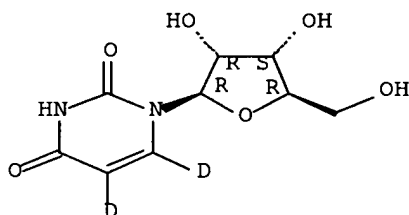
Ru

RN 7440-48-4 CAPLUS  
 CN Cobalt (CA INDEX NAME)

Co

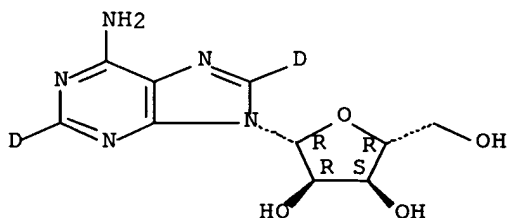
IT 40632-21-1P, Uridine-5,6-d2 82845-88-3P,  
 Adenosine-2,8-d2 96412-41-8P, Guanosine-8-d 697807-01-5P  
 , Inosine-2,8-d2  
 RL: IMF (Industrial manufacture); SPN (Synthetic  
 preparation); PREP (Preparation)  
 (method for deuteration or tritiation of heterocyclic compds.)  
 RN 40632-21-1 CAPLUS  
 CN Uridine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



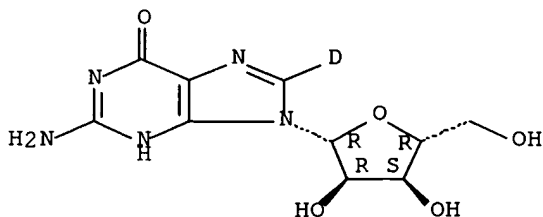
RN 82845-88-3 CAPLUS  
 CN Adenosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



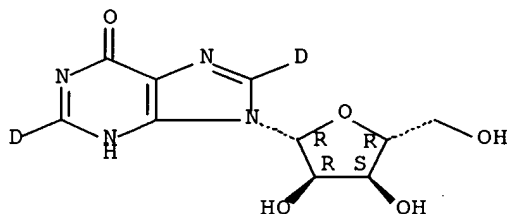
RN 96412-41-8 CAPLUS  
 CN Guanosine-8-d (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 697807-01-5 CAPLUS  
CN Inosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:231394 CAPLUS Full-text

DOCUMENT NUMBER: 140:406566

TITLE: Palladium-catalyzed H-D exchange reaction under hydrothermal condition

AUTHOR(S): Matsubara, Seiji; Yokota, Yutaka; Oshima, Koichiro

CORPORATE SOURCE: Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, 615-8510, Japan

SOURCE: Chemistry Letters (2004), 33(3), 294-295

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:406566

AB Alkenes and alkanes were converted into fully deuterium labeled ones by treatment with palladium on charcoal and deuterium oxide under hydrothermal condition. This simple method to get fully deuterium labeled compds. is easy to apply to various types of organic compds.

CC 24-6 (Alicyclic Compounds)

IT **Deuteration**

**Deuteration catalysts**

(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)

IT **7440-05-3, Palladium, uses**

RL: **CAT (Catalyst use); USES (Uses)**

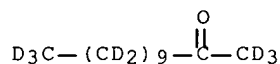
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)



IT 1486-01-7P 10249-89-5P, Cyclooctene-d14 16450-78-5P, Cyclododecane-d24  
 36340-20-2P, Pentadecane-d32 688320-41-4P 688320-42-5P,  
 Cyclopentadecane-d30 688320-43-6P, Cyclooctanone-d14 688320-44-7P,  
 Cyclodecanone-d18 688320-45-8P, Cyclododecanone-d22 688320-46-9P,  
 Cyclopentadecanone-d28 **688320-48-1P** 688320-49-2P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (palladium-catalyzed H-D exchange reaction under hydrothermal  
 conditions)  
 IT **7440-05-3**, Palladium, uses  
 RL: **CAT (Catalyst use); USES (Uses)**  
 (palladium-catalyzed H-D exchange reaction under hydrothermal  
 conditions)  
 RN 7440-05-3 CAPLUS  
 CN Palladium (CA INDEX NAME)

Pd

IT **688320-48-1P**  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (palladium-catalyzed H-D exchange reaction under hydrothermal  
 conditions)  
 RN 688320-48-1 CAPLUS  
 CN 2-Dodecanone-1,1,1,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-d24  
 (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:991461 CAPLUS Full-text  
 DOCUMENT NUMBER: 140:41620  
 TITLE: Process for deuteration of inert methylene  
 INVENTOR(S): Hirota, Kosaku; Sajiki, Hironao  
 PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 27 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	----	-----	-----
WO 2003104166	A1	20031218	WO 2002-JP11785	20021112
W: JP, US				
US 2005177015	A1	20050811	US 2004-516638	20041202
US 7126023	B2	20061024		
PRIORITY APPLN. INFO.:			JP 2002-166224	A 20020606
			WO 2002-JP11785	W 20021112

OTHER SOURCE(S): MARPAT 140:41620

AB The invention relates to a process for deuteration of inert alkanes with activated palladium-carbon, specifically, a process for deuterating a compound having either a Me group or an alkylene group having two or more carbon atoms in a state directly bonded to an optionally substituted aromatic ring through replacement of one or more hydrogen atoms of the Me group or one or more of the benzylic and other hydrogen atoms of the alkylene group by deuterium, characterized in that the above compound is subjected to refluxing in a closed system in the presence of activated palladium-carbon in a state dissolved in a deuterated solvent.

IC ICM C07B059-00

ICS C07M005-00

CC 21-2 (General Organic Chemistry)

IT **Deuteration****Deuteration catalysts**

(process for deuteration of inert methylene using activated palladium-carbon catalyst)

IT **7440-05-3**, Palladium, usesRL: **CAT (Catalyst use)**; USES (Uses)

(carbon-supported; process for deuteration of inert methylene using activated palladium-carbon catalyst)

IT 1124-18-1P 14202-49-4P 38729-11-2P 65087-58-3P 94367-56-3P

117637-87-3P, Benzenepropan- $\beta,\beta,\gamma,\gamma$ -d<sub>4</sub>-ol156310-21-3P **634897-72-6P** 634897-76-0P 634897-78-2P634897-80-6P 634897-82-8P 634897-84-0P **634897-86-2P**,Benzenepropanoic-d<sub>4</sub> acid-d **634897-88-4P**, Benzene-d<sub>5</sub>-butanoic-d<sub>6</sub>acid-d **634897-90-8P 634897-92-0P 634897-99-7P**634898-02-5P, Benzenebutan- $\beta,\beta,\gamma,\gamma,\delta,\delta$ -d<sub>6</sub>-ol 634898-04-7P, Benzenepentan- $\beta,\beta,\gamma,\gamma,\delta,$  $\delta,\epsilon,\epsilon$ -d<sub>8</sub>-ol 634898-08-1P 634898-10-5P

634898-14-9P 634898-16-1P 634898-20-7P 634898-23-0P 634898-25-2P

634898-29-6P 634898-34-3P

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(process for deuteration of inert methylene using activated palladium-carbon catalyst)

IT **7440-05-3**, Palladium, usesRL: **CAT (Catalyst use)**; USES (Uses)

(carbon-supported; process for deuteration of inert methylene using activated palladium-carbon catalyst)

RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

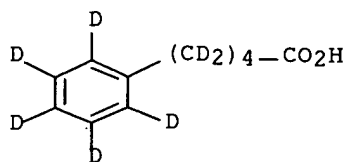
Pd

IT **634897-72-6P 634897-86-2P**, Benzenepropanoic-d<sub>4</sub> acid-d**634897-88-4P**, Benzene-d<sub>5</sub>-butanoic-d<sub>6</sub> acid-d **634897-90-8P****634897-92-0P 634897-99-7P**RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(process for deuteration of inert methylene using activated palladium-carbon catalyst)

RN 634897-72-6 CAPLUS

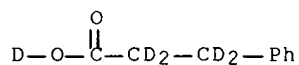
CN Benzene-d<sub>5</sub>-pentanoic-d<sub>8</sub> acid, sodium salt (9CI) (CA INDEX NAME)



● Na

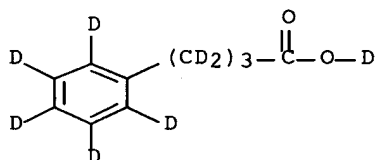
RN 634897-86-2 CAPLUS

CN Benzenepropanoic-d4 acid-d (9CI) (CA INDEX NAME)



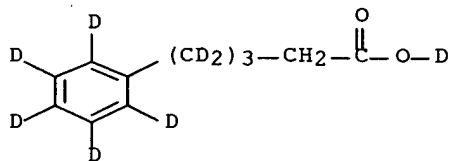
RN 634897-88-4 CAPLUS

CN Benzene-d5-butanoic-d6 acid-d (9CI) (CA INDEX NAME)



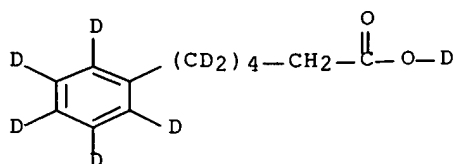
RN 634897-90-8 CAPLUS

CN Benzene-d5-pentanoic- $\beta, \beta, \gamma, \gamma, \delta, \delta$ -d6 acid-d (9CI) (CA INDEX NAME)

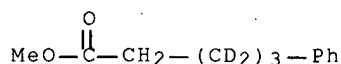


RN 634897-92-0 CAPLUS

CN Benzene-d5-hexanoic- $\beta, \beta, \gamma, \gamma, \delta, \delta, \epsilon, \epsilon$ -d8 acid-d (9CI) (CA INDEX NAME)



RN 634897-99-7 CAPLUS  
 CN Benzenepentanoic-β,β,γ,γ,δ,δ-d6 acid,  
 methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:474175 CAPLUS Full-text

DOCUMENT NUMBER: 139:395665

TITLE: Combining microwave-enhanced deuteration reactions with parallel synthesis procedures

AUTHOR(S): Chappelle, Michael R.; Harding, John R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.

CORPORATE SOURCE: Amersham Biosciences, The Maynard Centre, Cardiff, CF14 7YT, UK

SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 567-574

CODEN: JLCRD4; ISSN: 0362-4803

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:395665

AB The development of combined microwave-enhanced/parallel synthesis procedures and their application to the deuteration of organic compds. via examples of solid-state hydrogenation is reported. Other labeling procedures, such as solution state catalytic dehalogenations, hydrogenations as well as hydrogen isotope exchange reactions also benefit from the combined technol.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Debromination

Dechlorination

Dehalogenation

**Deuteration catalysts**

Microwave

Solid phase synthesis

(combining microwave-enhanced deuteration with parallel synthesis procedures)

IT **Deuteration**

Hydrogenation catalysts

(solid-state deuteration; combining microwave-enhanced deuteration with parallel synthesis procedures)

IT 3375-31-3 10049-07-7, Rhodium chloride (RhCl3)

RL: **CAT (Catalyst use)**; USES (Uses)

(combining microwave-enhanced deuteration with parallel synthesis procedures)

IT 10473-16-2P 16089-48-8P, 3-Phenyl-2-Propenoic acid potassium salt  
 36568-19-1P, 3-(4-Chlorophenyl)-2-Propenoic acid potassium salt  
 625383-67-7P, 3-(4-Bromophenyl)-2-propenoic acid potassium salt  
 625383-68-8P, 4-Bromobenzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid potassium salt  
**625383-69-9P**, 3-(Phenyl-4-d)-2-Propenoic acid potassium salt  
 625383-70-2P, 3-(3-Bromophenyl)-2-propenoic acid potassium salt  
 625383-72-4P **625383-73-5P**, 3-(Phenyl-3-d)-2-Propenoic acid potassium salt  
 625383-74-6P, 1-Bromo-4-(ethyl-1,2-d<sub>2</sub>)benzene  
 625383-75-7P, 3-(4-Fluorophenyl)-2-Propenoic acid potassium salt  
 625383-76-8P, 3-(2-Chlorophenyl)-2-Propenoic acid potassium salt  
 625383-77-9P, 3-(3-Chlorophenyl)-2-Propenoic acid potassium salt  
**625383-78-0P** 625383-80-4P, 4-Fluorobenzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid potassium salt  
 625383-82-6P, 2-Chlorobenzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid potassium salt  
 625383-84-8P, 3-Chlorobenzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid potassium salt  
 625383-86-0P, 4-Chlorobenzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid potassium salt  
 625383-88-2P, 1-Bromo-4-(ethenyl-1,2-d<sub>2</sub>)benzene  
 625383-90-6P

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(combining microwave-enhanced deuteration with parallel synthesis procedures)

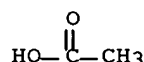
IT **3375-31-3 10049-07-7**, Rhodium chloride (RhCl<sub>3</sub>)

RL: **CAT (Catalyst use)**; USES (Uses)

(combining microwave-enhanced deuteration with parallel synthesis procedures)

RN 3375-31-3 CAPLUS

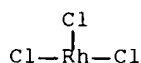
CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)



●1/2 Pd(II)

RN 10049-07-7 CAPLUS

CN Rhodium chloride (RhCl<sub>3</sub>) (CA INDEX NAME)



IT **625383-69-9P**, 3-(Phenyl-4-d)-2-Propenoic acid potassium salt

**625383-73-5P**, 3-(Phenyl-3-d)-2-Propenoic acid potassium salt

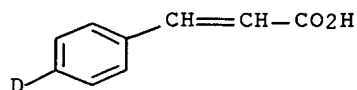
**625383-78-0P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(combining microwave-enhanced deuteration with parallel synthesis procedures)

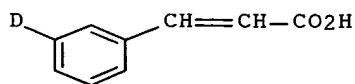
RN 625383-69-9 CAPLUS

CN 2-Propenoic acid, 3-(phenyl-4-d)-, potassium salt (9CI) (CA INDEX NAME)



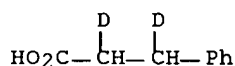
● K

RN 625383-73-5 CAPLUS  
 CN 2-Propenoic acid, 3-(phenyl-3-d)-, potassium salt (9CI) (CA INDEX NAME)



● K

RN 625383-78-0 CAPLUS  
 CN Benzenepropanoic- $\alpha,\beta$ -d<sub>2</sub> acid, potassium salt (9CI) (CA INDEX NAME)

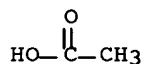


● K

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

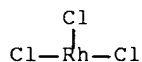
L19 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:483457 CAPLUS Full-text  
 DOCUMENT NUMBER: 138:4188  
 TITLE: Development of combined microwave-enhanced labelling procedures for maximizing deuterium incorporation  
 AUTHOR(S): Chapelle, Michael R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.  
 CORPORATE SOURCE: Amersham Plc, Cardiff Laboratories, Cardiff, CF14 7YT, UK  
 SOURCE: Tetrahedron Letters (2002), 43(29), 5117-5118  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:4188

- AB Combined hydrogenation/aromatic dehalogenation under microwave-enhanced conditions provides a rapid route to deuterium labeled compds. with enhanced isotopic incorporation.
- CC 21-2 (General Organic Chemistry)
- IT Debromination  
 Debromination catalysts  
 Dechlorination  
 Dechlorination catalysts  
**Deuteration**  
**Deuteration catalysts**  
 Hydrogenation  
 Hydrogenation catalysts  
 Microwave  
 (preparation of deuterium-labeled compds. with enhanced isotopic incorporation via rhodium- and palladium-catalyzed microwave-induced combined hydrogenation/aromatic dehalogenation procedure)
- IT **3375-31-3**, Palladium diacetate **10049-07-7**, Rhodium chloride (RhCl<sub>3</sub>)  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (microwave-induced rhodium- and palladium-catalyzed combined hydrogenation/aromatic dehalogenation routes for preparation of deuterium-labeled compds. with enhanced isotopic incorporation)
- IT **99532-30-6P** 477284-15-4P **477284-16-5P**,  
 Benzene-4-d-propanoic- $\alpha,\beta$ -d<sub>2</sub> acid  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (preparation of deuterium-labeled compds. with enhanced isotopic incorporation via combined microwave-induced hydrogenation/aromatic dehalogenation procedure)
- IT **477284-17-6P**, Benzene-3-d-propanoic- $\alpha,\beta$ -d<sub>2</sub> acid  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (preparation of deuterium-labeled compds. with enhanced isotopic incorporation via microwave-induced hydrogenation/aromatic dehalogenation procedure)
- IT **3375-31-3**, Palladium diacetate **10049-07-7**, Rhodium chloride (RhCl<sub>3</sub>)  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (microwave-induced rhodium- and palladium-catalyzed combined hydrogenation/aromatic dehalogenation routes for preparation of deuterium-labeled compds. with enhanced isotopic incorporation)
- RN 3375-31-3 CAPLUS
- CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)

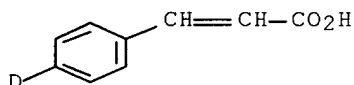


●1/2 Pd(II)

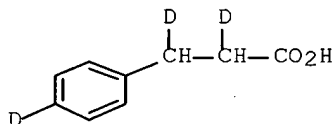
- RN 10049-07-7 CAPLUS
- CN Rhodium chloride (RhCl<sub>3</sub>) (CA INDEX NAME)



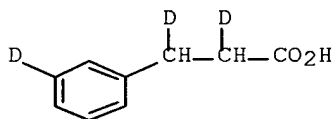
IT 99532-30-6P 477284-16-5P, Benzene-4-d-propanoic-  
 $\alpha,\beta$ -d2 acid  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of deuterium-labeled compds. with enhanced isotopic  
 incorporation via combined microwave-induced hydrogenation/aromatic  
 dehalogenation procedure)  
 RN 99532-30-6 CAPLUS  
 CN 2-Propenoic acid, 3-(phenyl-4-d)- (9CI) (CA INDEX NAME)



RN 477284-16-5 CAPLUS  
 CN Benzene-4-d-propanoic- $\alpha,\beta$ -d2 acid (9CI) (CA INDEX NAME)



IT 477284-17-6P, Benzene-3-d-propanoic- $\alpha,\beta$ -d2 acid  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of deuterium-labeled compds. with enhanced isotopic  
 incorporation via microwave-induced hydrogenation/aromatic dehalogenation  
 procedure)  
 RN 477284-17-6 CAPLUS  
 CN Benzene-3-d-propanoic- $\alpha,\beta$ -d2 acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:550049 CAPLUS Full-text  
 DOCUMENT NUMBER: 133:322037  
 TITLE: Deuteration of estrogens using Pd/C as a catalyst  
 AUTHOR(S): Kiuru, Paula; Wahala, Kristiina  
 CORPORATE SOURCE: Department of Chemistry, Organic Chemistry Laboratory,



## SOURCE:

University of Helsinki, FIN-00014, Finland  
 Synthesis and Applications of Isotopically Labelled  
 Compounds 1997, Proceedings of the International  
 Symposium, 6th, Philadelphia, PA, United States, Sept.  
 14-18, 1997 (1998), Meeting Date 1997, 475-477.  
 Editor(s): Heys, J. Richard; Melillo, David G. John  
 Wiley & Sons Ltd.: Chichester, UK.  
 CODEN: 69AGFQ

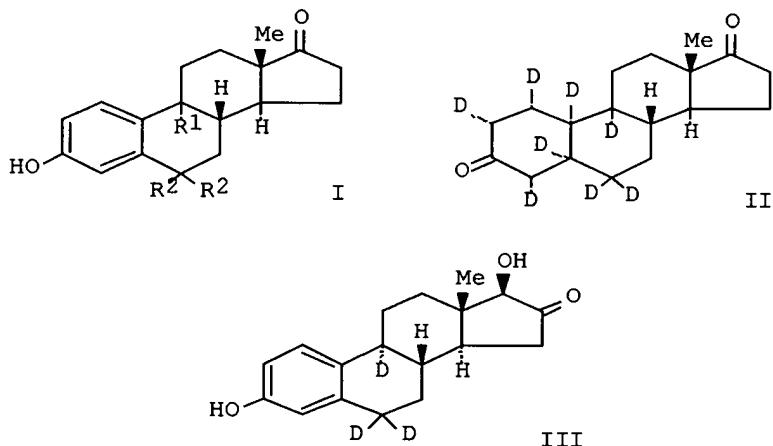
## DOCUMENT TYPE:

Conference

## LANGUAGE:

English

GI



AB The reduction of estrone (I; R1 = R2 = H) using D2 on Pd/C gives  
 1α,2α,4α,5α,6,6,9α,10α-[2H3]estrane-3,17-dione (II), the configuration of  
 deuteriums been established by NMR. Pd/C catalyzes the H-D exchange also at  
 the benzylic positions of estrogens. 6,6,9-[2H3]estrone (I; R1 = R2 = D) and  
 6,6,9-[2H3]-16-ketoestradiol (III) were synthesized in high isotopic purity.

CC 32-3 (Steroids)

IT Absolute configuration

**Deuteration****Deuteration catalysts**

(stereoselective deuteration of estrogens using palladium/carbon as a  
 catalyst)

IT **7440-05-3D**, Palladium, on carbon, uses

RL: **CAT (Catalyst use)**; USES (Uses)

(stereoselective deuteration of estrogens using palladium/carbon as a  
 catalyst)

IT 50888-33-0P, 6,6,9-[2H3]Estrone 303128-11-2P,

1α,5α,6,6,9α,10α-[2H6]Estrane-3,17-dione

**303128-12-3P**, 6,6,9-[2H3]-16-Ketoestradiol

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(stereoselective deuteration of estrogens using palladium/carbon as a  
 catalyst)

IT **7440-05-3D**, Palladium, on carbon, uses

RL: **CAT (Catalyst use)**; USES (Uses)

(stereoselective deuteration of estrogens using palladium/carbon as a  
 catalyst)

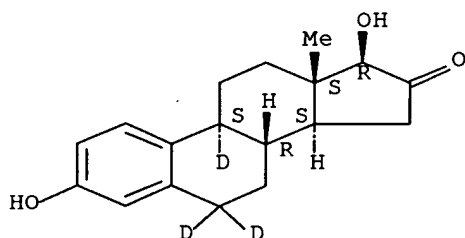
RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

IT **303128-12-3P**, 6,6,9-[2H3]-16-Ketoestradiol  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (stereoselective deuteration of estrogens using palladium/carbon as a catalyst)  
 RN 303128-12-3 CAPLUS  
 CN Estra-1,3,5(10)-trien-16-one-6,6,9-d3, 3,17-dihydroxy-, (17 $\beta$ )- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



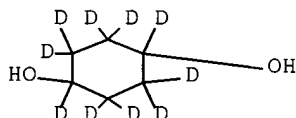
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:549991 CAPLUS Full-text  
 DOCUMENT NUMBER: 134:147329  
 TITLE: Convenient synthesis of deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide  
 AUTHOR(S): Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi  
 CORPORATE SOURCE: Center of Advanced Instrumental Analysis, Kyushu University, Kasuga, 816, Japan  
 SOURCE: Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 203-206.  
 Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.  
 CODEN: 69AGFQ  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:147329  
 AB A symposium report on the deuteration of polyhalophenolic substrates in the presence of nickel-aluminum alloy.  
 CC 24-5 (Alicyclic Compounds)  
 Section cross-reference(s): 34  
 IT **Deuteration**  
**Deuteration catalysts**  
 (deuterated cycloalkanes from polyhalophenols with nickel-aluminum

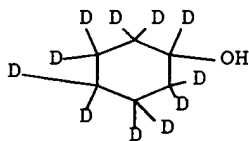
alloy in alkaline deuterium oxide)  
 IT **11114-68-4**  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)  
 IT **77787-72-5P 93131-17-0P, Cyclohexan-d11-ol**  
**324520-34-5P 324520-35-6P 324520-36-7P**  
 RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)  
 (deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)  
 IT **11114-68-4**  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)  
 RN 11114-68-4 CAPLUS  
 CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

Component	Component Registry Number
Al	7429-90-5
Ni	7440-02-0

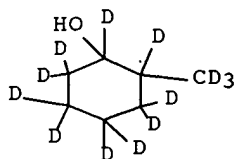
IT **77787-72-5P 93131-17-0P, Cyclohexan-d11-ol**  
**324520-34-5P 324520-35-6P 324520-36-7P**  
 RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)  
 (deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)  
 RN 77787-72-5 CAPLUS  
 CN 1,4-Cyclohexane-1,2,2,3,3,4,5,5,6,6-d10-diol (9CI) (CA INDEX NAME)



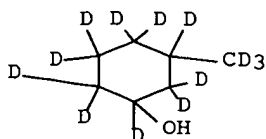
RN 93131-17-0 CAPLUS  
 CN Cyclohexan-d11-ol (9CI) (CA INDEX NAME)



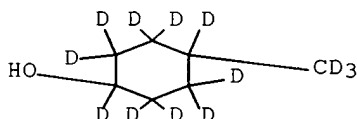
RN 324520-34-5 CAPLUS  
 CN Cyclohexan-1,2,2,3,3,4,4,5,5,6-d10-ol, 6-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 324520-35-6 CAPLUS  
 CN Cyclohexan-1,2,2,3,3,4,4,5,6,6-d10-ol, 5-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 324520-36-7 CAPLUS  
 CN Cyclohexan-1,2,2,3,3,4,5,5,6,6-d10-ol, 4-(methyl-d3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:414551 CAPLUS Full-text  
 DOCUMENT NUMBER: 133:192893  
 TITLE: Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst  
 AUTHOR(S): Papp, Eva; Banyai, Istvan; Joo, Ferenc  
 CORPORATE SOURCE: Research Group of Homogeneous Catalysis, Hungarian Academy of Sciences, Debrecen, H-4010, Hung.  
 SOURCE: Reaction Kinetics and Catalysis Letters (2000), 69(1), 23-30  
 CODEN: RKCLAU; ISSN: 0304-4122  
 PUBLISHER: Akademiai Kiado  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Hydrogenations in aqueous systems with the soluble [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst resulted in extensive deuteration of crotonic, trans-2-pentenoic and itaconic acids regardless of whether the deuterium source was D<sub>2</sub> or D<sub>2</sub>O. Itaconic acid was deuterated up to 3.6 D/methylsuccinic

acid. Detailed <sup>1</sup>H- and <sup>13</sup>C-NMR studies identified six isotopomers of the deuterated methylsuccinic acid product and revealed an important role of the H/D exchange on the catalytically active Pd-intermediate.

CC 23-16 (Aliphatic Compounds)

IT **Deuteration**

**Deuteration catalysts**

Hydrogenation

Hydrogenation catalysts

(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst)

IT **74091-55-7**

RL: **CAT (Catalyst use); USES (Uses)**

(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst)

IT 498-21-5P 169127-02-0P **289679-94-3P**, Butanoic-d acid

**289679-95-4P**, Pentanoic-d acid 289679-96-5P 289679-97-6P

289679-98-7P 289679-99-8P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst)

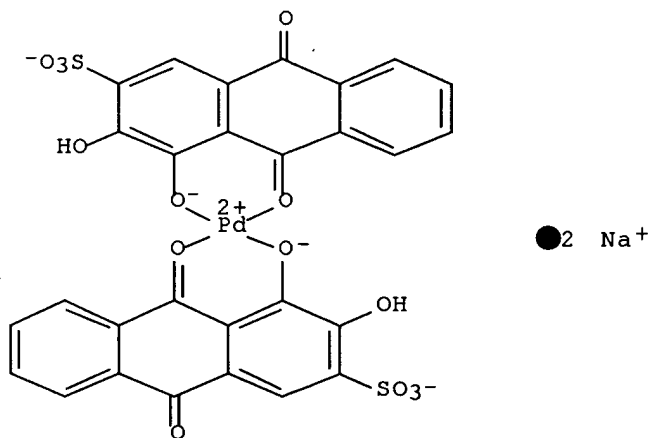
IT **74091-55-7**

RL: **CAT (Catalyst use); USES (Uses)**

(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst)

RN 74091-55-7 CAPLUS

CN Palladate(2-), bis[9,10-dihydro-3-hydroxy-4-(hydroxy-κO)-9-oxo-10-(oxo-κO)-2-anthracenesulfonato(2-)]-, disodium (9CI) (CA INDEX NAME)



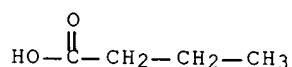
IT **289679-94-3P**, Butanoic-d acid **289679-95-4P**, Pentanoic-d acid

RL: **SPN (Synthetic preparation); PREP (Preparation)**

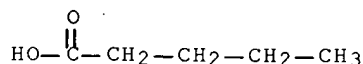
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)<sub>2</sub>] catalyst)

RN 289679-94-3 CAPLUS

CN Butanoic-d acid (9CI) (CA INDEX NAME)



RN 289679-95-4 CAPLUS  
 CN Pentanoic-d acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:324308 CAPLUS Full-text

DOCUMENT NUMBER: 127:17291

TITLE: First Evidence That the Mechanism of Catalytic Hydrogenation with Homogeneous Palladium and Rhodium Catalysts Is Strongly Influenced by Substrate Polarity

AUTHOR(S): Yu, Jinqun; Spencer, Jonathan B.

CORPORATE SOURCE: University Chemical Laboratory, University of Cambridge, Cambridge, CB2 1EW, UK

SOURCE: Journal of the American Chemical Society (1997), 119(22), 5257-5258

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have observed that when cis-alkenes are hydrogenated with homogeneous palladium and rhodium catalysts they readily isomerize to the trans-configuration with the incorporation of a deuterium atom. By studying how electron withdrawing and donating groups conjugated to the double bond influence the location of deuterium addition we have been able to gain a clear insight into how the metal hydrogen bond in the catalyst is polarized just prior to adding to the cis-alkene. Remarkably, the result demonstrate that the palladium hydrogen bond is capable of being polarized in either mode (a  $\text{Pd}\delta^+-\text{H}\delta^-$  or b  $\text{Pd}\delta^--\text{H}\delta^+$ ) depending on the coulombic properties of the substrate, whereas the rhodium catalyst studied is dominated by mode a ( $\text{Rh}\delta^+-\text{H}\delta^-$ ). This provides strong evidence that the mechanism of catalytic hydrogenation is a 2 electron process that can be dramatically affected by the substrate's polarity.

CC 22-7 (Physical Organic Chemistry)  
 Section cross-reference(s): 29, 67

IT Conjugation (bond)

#### Deuteration

#### Deuteration catalysts

Electron transfer

Hydrogenation

Hydrogenation catalysts

Isomerization

Isomerization catalysts

NMR (nuclear magnetic resonance)

Regiochemistry

## Resonance

## Substituent effects

(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

- IT **14694-95-2**, Chlorotris(triphenylphosphine)rhodium  
**31277-98-2**, Bis[1,2-bis(diphenylphosphino)ethane]palladium  
 RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

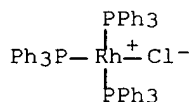
- IT 107-93-7P 140-10-3P, preparation 623-43-8P 943-89-5P 1005-64-7P  
 1011-54-7P 4747-15-3P **69104-43-4P** 89039-12-3P 89039-13-4P  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

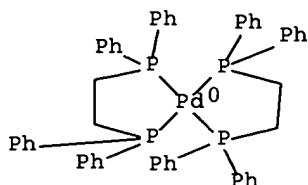
- IT **14694-95-2**, Chlorotris(triphenylphosphine)rhodium  
**31277-98-2**, Bis[1,2-bis(diphenylphosphino)ethane]palladium  
 RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

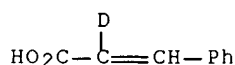
- RN 14694-95-2 CAPLUS  
 CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



- RN 31277-98-2 CAPLUS  
 CN Palladium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]-, (T-4)- (9CI) (CA INDEX NAME)



- IT **69104-43-4P**  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)  
 RN 69104-43-4 CAPLUS  
 CN 2-Propenoic-2-d acid, 3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:98985 CAPLUS Full-text

DOCUMENT NUMBER: 124:260517

TITLE: Retention of optical purity in H-D exchange reactions catalyzed by cobalt-aluminum alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O

AUTHOR(S): Mukumoto, Mamoru; Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi; Tsukinoki, Takehito; Nagano, Yoshiaki

CORPORATE SOURCE: Dep. Mol. Sci. Technol., Kyushu Univ., Kasuga, 816, Japan

SOURCE: Chemistry Letters (1996), (2), 165-6  
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:260517

AB Co-Al alloy in a sodium carbonate-deuterium oxide solution catalyzes the H-D exchange reaction of optically active benzylic hydrogen atom without racemization. Thus, (R)-mandelic acid give Me α-D-(R)-mandelate in 89% yield with 99% enantiomeric excess.

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Deuteration catalysts**

(stereoselective; deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

IT **Deuteration**

(stereoselective, deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

IT **11114-55-9**

RL: **CAT (Catalyst use); USES (Uses)**

(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

IT 175289-31-3P **175289-32-4P** 175289-33-5P 175289-34-6P  
175289-35-7P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

IT **11114-55-9**

RL: **CAT (Catalyst use); USES (Uses)**

(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

RN 11114-55-9 CAPLUS

CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

Component	Component Registry Number
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Al	7429-90-5
Co	7440-48-4

IT **175289-32-4P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**

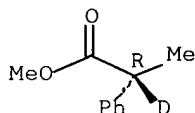


(deuteration of benzylic compds. with retention of configuration using  
Co-Al alloy in Na<sub>2</sub>CO<sub>3</sub>-D<sub>2</sub>O)

RN 175289-32-4 CAPLUS

CN Benzeneacetic-d acid,  $\alpha$ -methyl-, methyl ester, (R)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



L19 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:231056 CAPLUS Full-text

DOCUMENT NUMBER: 110:231056

TITLE: Homogeneous deuteration of alkenes using  
[RhCl(4R,5R-diop)] catalysts

AUTHOR(S): Gungor, Muammer; Jardine, Fred H.; Wheatley, J. Denis  
CORPORATE SOURCE: Dep. Phys. Sci., North East London Polytech., London,  
E15 4LZ, UK

SOURCE: Polyhedron (1988), 7(19-20), 1827-9  
CODEN: PLYHDE; ISSN: 0277-5387

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mass spectrometric analyses of the products from the homogeneous deuteration of alkenes using the title (4R,5R- DIOP)/{[RhCl(cyclooctene)<sub>2</sub>]<sub>2</sub>} catalyst system show that considerable quantities of polydeuterated products are obtained. These products arise from the decomposition of the intermediate rhodium(III)alkyl complex [RhDCl(alkyl)(DIOP)] before the second atom of deuterium can be transferred to the alkyl ligand. Its decomposition by  $\beta$ -hydride abstraction brings about both polydeuteration and scrambled addition of deuterium to the alkene. The yields of specifically deuterated products are inferior to those obtained from Wilkinson-type catalysts. The best yields of dideuterated products are obtained from substituted alkenes that chelate to the catalyst and thereby stabilize the intermediate alkyl. The preparation of a threitol ditosylate intermediate in dry pyridine was noted for its dangerous exothermicity.

CC 23-2 (Aliphatic Compounds)  
Section cross-reference(s): 24, 25

IT **Deuteration**  
(of alkenes, mechanism of catalytic)

IT **Deuteration catalysts**  
(rhodium-DIOP complex, for alkenes)

IT **12279-09-3**  
RL: **CAT (Catalyst use)**; **USES (Uses)**  
(catalysts, containing DIOP, for deuteration of alkenes)

IT **66502-82-7P**  
RL: **PRP (Properties)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**  
(preparation and carbon-13 NMR of)

IT 292-64-8P, Cyclooctane 24588-43-0P, Octane-1,2-d<sub>2</sub> 33283-80-6P,  
Bicyclo[2.2.1]heptane-2,3-d<sub>2</sub> 71501-04-7P, Octane-d 73811-48-0P  
86812-02-4P, Cyclooctane-d 92475-64-4P, Hexane-1,2-d<sub>2</sub> 95236-97-8P,  
Heptane-1,2-d<sub>2</sub> 95237-00-6P 98821-91-1P, Cyclohexane-1,2-d<sub>2</sub>

118296-70-1P, Octane-1,2,?-d3 118296-71-2P, Octane-1,2,?,?-d4  
 118297-06-6P 118297-07-7P 118297-11-3P, Heptane-d 118297-12-4P,  
 Heptane-1,2,?-d3 118297-17-9P, Hexane-1,2,?-d3 118297-18-0P,  
 Hexane-1,2,?,?-d4 120625-93-6P, Cyclohexanone-2,3-d2 120625-94-7P,  
 Cyclooctane-1,2-d2 120625-95-8P 120625-96-9P **120625-97-0P**,  
 2-Hexanone-5,6-d2 120625-98-1P, Cyclohexane-1,2,?-d3 120625-99-2P,  
 Cyclohexanone-2,3,?-d3 120626-00-8P, Cyclooctane-1,2,?-d3 120626-01-9P  
 120626-02-0P **120626-03-1P** 120626-04-2P, Cyclooctane-1,2,?,?-d4  
**120626-05-3P**

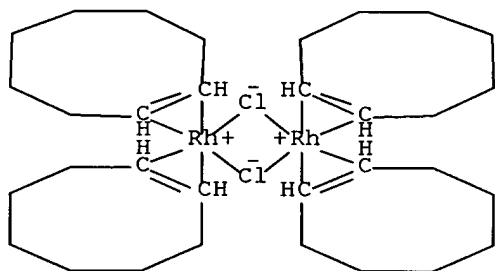
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (preparation of)

IT **12279-09-3**

RL: **CAT (Catalyst use); USES (Uses)**  
 (catalysts, containing DIOP, for deuteration of alkenes)

RN 12279-09-3 CAPLUS

CN Rhodium, di- $\mu$ -chlorotetrakis[(1,2- $\eta$ )-cyclooctene]di- (CA INDEX  
 NAME)



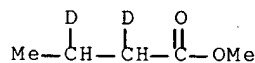
IT **66502-82-7P**

RL: PRP (Properties); **SPN (Synthetic preparation); PREP (Preparation)**

(preparation and carbon-13 NMR of)

RN 66502-82-7 CAPLUS

CN Butanoic-2,3-d2 acid, methyl ester (CA INDEX NAME)



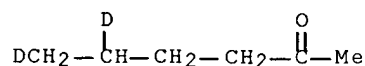
IT **120625-97-0P**, 2-Hexanone-5,6-d2 **120626-03-1P**

**120626-05-3P**

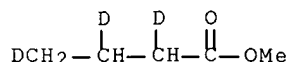
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (preparation of)

RN 120625-97-0 CAPLUS

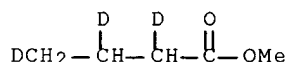
CN 2-Hexanone-5,6-d2 (9CI) (CA INDEX NAME)



RN 120626-03-1 CAPLUS  
 CN Butanoic-2,3,4-d3 acid, methyl ester (9CI) (CA INDEX NAME)



RN 120626-05-3 CAPLUS  
 CN Butanoic-2,3,4,?-d4 acid, methyl ester (9CI) (CA INDEX NAME)



L19 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:545159 CAPLUS Full-text

DOCUMENT NUMBER: 97:145159

ORIGINAL REFERENCE NO.: 97:24193a,24196a

TITLE: Some stereochemical characteristics of C-1H-C-2H exchange-reactions with Raney nickel catalyst in deuterium oxide

AUTHOR(S): Balza, Felipe; Perlin, Arthur S.

CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3C 3G1, Can.

SOURCE: Carbohydrate Research (1982), 107(2), 270-8

CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In C-deuteration of carbohydrates with Raney Ni in D2O, the following reaction-characteristics were observed: (a) at least 2 OH groups, not necessarily contiguous, are required for 1H-2H exchange to occur; (b) the rate of isotope incorporation into alkyl glycopyranosides is relatively slow when the C-H bond undergoing exchange is syn-axial with respect to an alkoxy group or when the bond is axial and vicinal to an equatorial alkoxy group; (c) an increase in the size of the alkoxy substituent leads to further diminution in the rate of exchange; (d) an equatorial H atom undergoes exchange more readily than an axial one; and (e) isotope exchange proceeds primarily with retention of configuration, although some degree of isomerization is almost always observed

CC 33-1 (Carbohydrates)

Section cross-reference(s): 22

IT **Deuteration catalysts**

(nickel, for carbohydrates)

IT **Deuteration**

(of carbohydrates over Raney nickel)

IT **7440-02-0**, uses and miscellaneous

RL: **CAT (Catalyst use)**; USES (Uses)

(catalysts, for deuteration of carbohydrates)

IT 68922-38-3P **83158-38-7P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(preparation of)

IT **7440-02-0**, uses and miscellaneous

RL: **CAT (Catalyst use)**; USES (Uses)

(catalysts, for deuteration of carbohydrates)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

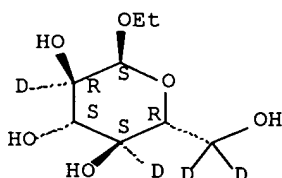
IT 83158-38-7P

RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(preparation of)

RN 83158-38-7 CAPLUS

CN  $\alpha$ -D-Glucopyranoside-2,4,6,6-C-d<sub>4</sub>, ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:461411 CAPLUS Full-text

DOCUMENT NUMBER: 95:61411

ORIGINAL REFERENCE NO.: 95:10371a,10374a

TITLE: A versatile procedure for the preparation of palmitic acid-d<sub>2</sub> and stearic acid-d<sub>6</sub>

AUTHOR(S): Adlof, R. O.; Emken, E. A.

CORPORATE SOURCE: North. Reg. Res. Cent., USDA, Peoria, IL, 61604, USA

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(3), 419-26

CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 95:61411

AB Me(CH<sub>2</sub>)<sub>3</sub>(CD<sub>2</sub>)<sub>2</sub>(CHD)<sub>2</sub>(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>H and Me(CH<sub>2</sub>)<sub>5</sub>(CHD)<sub>2</sub>(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>H were prepared from the corresponding 9,10-unsatd. Me esters by catalytic deuteration [(Ph<sub>3</sub>P)<sub>3</sub>RhCl, C<sub>6</sub>H<sub>6</sub>, under D, overnight) and saponification (KOH, aqueous MeOH, under N, reflux, 1.5). Me(CH<sub>2</sub>)<sub>5</sub>CH:CH(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>Me was prepared (65%) by Wittig reaction of [Me(CH<sub>2</sub>)<sub>6</sub>Ph<sub>3</sub>P]<sup>+</sup>I<sup>-</sup> with OHC(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>Me (DMF, NaOMe, 11°, overnight).

CC 23-16 (Aliphatic Compounds)

IT **Deuteration**

(of unsatd. fatty acid esters, rhodium-catalyzed)

IT **Deuteration catalysts**

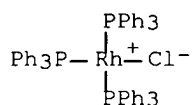
(tris(triphenylphosphine)chlororhodium, for unsatd. fatty acids)

IT **14694-95-2**RL: **CAT (Catalyst use); USES (Uses)**

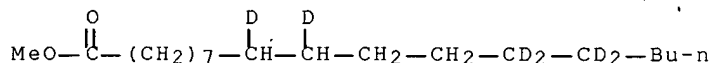
(catalysts, for deuteration of unsatd. fatty acids)

IT **78387-67-4P 78387-69-6P**RL: **RCT (Reactant); SPN (Synthetic preparation); PREP**

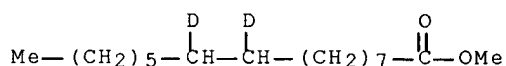
(Preparation); RACT (Reactant or reagent)  
 (preparation and saponification of)  
 IT 78387-68-5P 78387-70-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 14694-95-2  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, for deuteration of unsatd. fatty acids)  
 RN 14694-95-2 CAPLUS  
 CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



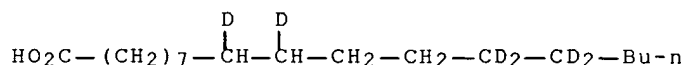
IT 78387-67-4P 78387-69-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and saponification of)  
 RN 78387-67-4 CAPLUS  
 CN Octadecanoic-9,10,13,13,14,14-d6 acid, methyl ester (9CI) (CA INDEX NAME)



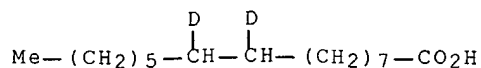
RN 78387-69-6 CAPLUS  
 CN Hexadecanoic-9,10-d2 acid, methyl ester (9CI) (CA INDEX NAME)



IT 78387-68-5P 78387-70-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 78387-68-5 CAPLUS  
 CN Octadecanoic-9,10,13,13,14,14-d6 acid (9CI) (CA INDEX NAME)



RN 78387-70-9 CAPLUS  
 CN Hexadecanoic-9,10-d2 acid (9CI) (CA INDEX NAME)



L19 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:139371 CAPLUS Full-text

DOCUMENT NUMBER: 86:139371

ORIGINAL REFERENCE NO.: 86:21873a,21876a

TITLE: Molecular hydrogenation, deuteration and oxygenation

AUTHOR(S): Khan, N. A.; Ahmed, R.

CORPORATE SOURCE: BCSIR Lab., Chittagong, Bangladesh

SOURCE: Bangladesh Journal of Scientific and Industrial

Research (1976), 11(1-4), 148-53

CODEN: BJSIBL; ISSN: 0304-9809

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Four acetylenic compds. and Me linoleate were hydrogenated and deuterated using H and D containing Ni W8, W9, and W10 catalysts, e.g., Me(CH<sub>2</sub>)<sub>7</sub>C.tplbond.C(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>Me gave Me(CH<sub>2</sub>)<sub>7</sub>CH:CH(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>Me and Me(CH<sub>2</sub>)<sub>7</sub>CD:CD(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>Me. Oxygenation of the reduced products showed that the deuterio-compds. have higher induction period than the corresponding H compds.

CC 23-17 (Aliphatic Compounds)

IT **Deuteration catalysts**

Hydrogenation catalysts

(nickel, for acetylenic compds. and methyl linolenate)

IT **Deuteration**

Hydrogenation

(of acetylenic compds. and methyl linolenate)

IT **7440-02-0**, uses and miscellaneous

RL: **CAT (Catalyst use)**; USES (Uses)

(catalysts, for hydrogenation and deuteration of acetylenic compds. and methyl linolenate)

IT 2462-84-2P 2462-85-3P 5557-31-3P **56554-40-6P**

**62439-46-7P** 62439-47-8P 62439-48-9P 62439-49-0P

**62439-50-3P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(preparation and oxygenation of)

IT **7440-02-0**, uses and miscellaneous

RL: **CAT (Catalyst use)**; USES (Uses)

(catalysts, for hydrogenation and deuteration of acetylenic compds. and methyl linolenate)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

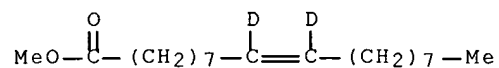
IT **56554-40-6P 62439-46-7P 62439-50-3P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(preparation and oxygenation of)

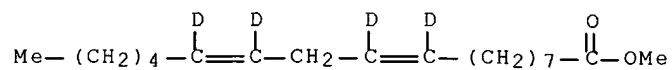
RN 56554-40-6 CAPLUS

CN 9-Octadecenoic-9,10-d<sub>2</sub> acid, methyl ester (9CI) (CA INDEX NAME)



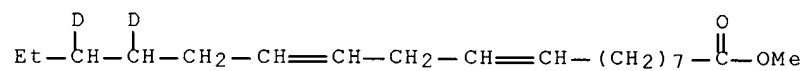
RN 62439-46-7 CAPLUS

CN 9,12-Octadecadienoic-9,10,12,13-d4 acid, methyl ester (9CI) (CA INDEX NAME)



RN 62439-50-3 CAPLUS

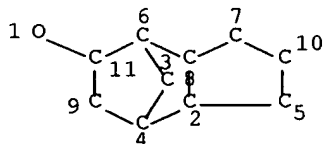
CN 9,12-Octadecadienoic-15,16-d2 acid, methyl ester (9CI) (CA INDEX NAME)



## Compound of Claim 12:

=&gt; d que 132

L25 3 SEA FILE=REGISTRY ABB=ON PLU=ON 13380-89-7/CRN  
 L26 2 SEA FILE=CAPLUS ABB=ON PLU=ON L25  
 L27 STR



## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

## STEREO ATTRIBUTES: NONE

L28 52 SEA FILE=REGISTRY FAM FUL L27  
 L29 133 SEA FILE=CAPLUS ABB=ON PLU=ON L28  
 L30 168165 SEA FILE=CAPLUS ABB=ON PLU=ON ?DEUTER?  
 L31 4 SEA FILE=CAPLUS ABB=ON PLU=ON L29 AND L30  
 L32 6 SEA FILE=CAPLUS ABB=ON PLU=ON L31 OR L26

=&gt; d 132 ibib abs hitind hitstr tot

L32 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:589514 CAPLUS Full-text

DOCUMENT NUMBER: 141:139883

TITLE: Method of catalytic **deuteration** of carbonyl compounds or secondary alcohols by heavy water

INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao

PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060831	A1	20040722	WO 2003-JP14182	20031107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,				



KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2511885	A1	20040722	CA 2003-2511885	20031107
AU 2003277596	A1	20040729	AU 2003-277596	20031107
EP 1577280	A1	20050921	EP 2003-814536	20031107

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

CN 1732135	A	20060208	CN 2003-80107483	20031107
US 2006116535	A1	20060601	US 2005-539188	20050616
IN 2005KN01449	A	20070720	IN 2005-KN1449	20050726

PRIORITY APPLN. INFO.:  
 JP 2002-378932 A 20021227  
 WO 2003-JP14182 W 20031107

OTHER SOURCE(S): CASREACT 141:139883; MARPAT 141:139883

AB Described is a method of **deuterating** a carbonyl or secondary alc. compound represented by the general formula R1-X-R2 (I) (wherein R1 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aralkyl ; R2 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aryl, aralkyl, alkoxy, aryloxy, hydroxy; X carbonyl, hydroxymethylene), which comprises reacting the compound represented by the general formula I with a **deuterium** source, in particular D2O, in the presence of a catalyst selected among activated palladium, platinum, rhodium, ruthenium, nickel, and cobalt catalysts. By the method, **deuteration**, which has been conducted under severe conditions, can be conducted under neutral conditions. Even when the compound contains an unsatd. bond, it can be **deuterated** without reducing the unsatd. bond. Not only hydrogens near the carbonyl or hydroxymethylene group but also those remotely situated from these groups are selectively **deuterated** without **deuterating** the carbon-carbon double or triple bonds. Thus, 500 mg tricyclo[5.2.1.02'6]decan-8-ol and 100 mg Pd-C were suspended in 17 mL D2O, purged with H, and heated at 180° for 24 h in an oil bath to give tricyclo[5.2.1.02'6]decan-8-ol **deuterated** by 96% at 8-position and 88% at other positions.

IC ICM C07B059-00

ICS C07C029-00; C07C031-02; C07C035-08; C07C035-29; C07C035-37;  
 C07C045-00; C07C049-04; C07C049-08; C07C049-433; C07C049-453;  
 C07C051-00; C07C053-10; C07C053-124; C07C057-04; C07M005-00

CC 21-2 (General Organic Chemistry)

ST **deuterated** carbonyl compd secondary alc prepn; catalytic **deuteration** ketone carboxylic acid secondary alc; palladium platinum **deuteration** catalyst; heavy water **deuteration** carbonyl compd secondary alc

IT **Deuteration**

**Deuteration** catalysts

(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT Carbonyl compounds (organic), reactions

Carboxylic acids, reactions

Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalytic **deuteration** of carbonyl compds. or secondary alc.

compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT Alcohols, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(secondary; catalytic **deuteration** of carbonyl compds. or

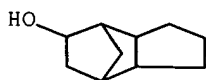
secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 7440-02-0, Raney nickel, uses

RL: CAT (Catalyst use); USES (Uses)

(catalysts; catalytic **deuteration** of carbonyl compds. or

- secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)
- IT 7440-05-3, Palladium, uses 7440-05-3D, Palladium, supported on carbon  
 7440-06-4, Platinum, uses 7440-06-4D, Platinum, supported on carbon  
 7440-16-6, Rhodium, uses 7440-16-6D, Rhodium, supported on alumina  
 7440-16-6D, Rhodium, supported on carbon 7440-18-8, Ruthenium, uses  
 7440-18-8D, Ruthenium, supported on carbon 7440-48-4, Cobalt, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalytic **deuteration** of carbonyl compds. or secondary alc.  
 compds. with heavy water in presence of palladium, platinum, rhodium,  
 ruthenium, or nickel)
- IT 67-64-1, Acetone, reactions 78-93-3, 2-Butanone, reactions 79-31-2,  
 Isobutyric acid 79-41-4, Methacrylic acid, reactions 106-35-4,  
 3-Heptanone 108-93-0, Cyclohexanol, reactions 108-94-1, Cyclohexanone,  
 reactions 110-43-0, 2-Heptanone 123-19-3, 4-Heptanone 127-09-3,  
 Sodium acetate 497-38-1, 2-Norbornanone 543-49-7, 2-Heptanol  
 589-55-9, 4-Heptanol 3385-61-3, Tricyclo[5.2.1.0<sup>2,6</sup>]-3-decen-8-ol  
 5536-61-8, Sodium methacrylate 7789-20-0, Water-d<sub>2</sub> **13380-89-7**,  
 Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-ol 13380-94-4, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-  
 one 63870-91-7, Norbornenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (catalytic **deuteration** of carbonyl compds. or secondary alc.  
 compds. with heavy water in presence of palladium, platinum, rhodium,  
 ruthenium, or nickel)
- IT 79-31-2DP, Isobutyric acid, **deuterated** 108-93-0DP,  
 Cyclohexanol, **deuterated** 666-52-4P, 2-Propanone-1,1,1,3,3,3-d<sub>6</sub>  
**13380-89-7DP**, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-ol, **deuterated**  
 14044-94-1P 18153-61-2DP, Bicyclo[2.2.1]heptan-2-one-3,3-d<sub>2</sub>,  
**deuterated** 21273-02-9DP, Cyclohexan-1-d-ol, **deuterated**  
 51209-49-5P, Cyclohexanone-d<sub>10</sub> 53481-06-4P 55935-44-9P 63870-91-7DP,  
 Norbornenol, **deuterated** 64118-21-4P 91468-78-9DP,  
 Bicyclo[2.2.1]heptan-2-d-2-ol, **deuterated** 350820-09-6P  
 725242-18-2P, 4-Heptanone-d<sub>14</sub> 725242-19-3DP, **deuterated**  
 725242-21-7DP, **deuterated** 725242-22-8P, 2-Heptanone-d<sub>14</sub>  
 725242-23-9P, 3-Heptanone-d<sub>14</sub> 725242-24-0P, 2-Heptanol-d<sub>15</sub>  
 725242-25-1P, 4-Heptanol-d<sub>15</sub> 725242-26-2DP, **deuterated**  
 725242-27-3DP, **deuterated** 725242-28-4DP, **deuterated**  
**725242-29-5DP, deuterated 725242-29-5P**  
**725242-30-8P** 725242-31-9P 725242-32-0DP, **deuterated**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (catalytic **deuteration** of carbonyl compds. or secondary alc.  
 compds. with heavy water in presence of palladium, platinum, rhodium,  
 ruthenium, or nickel)
- IT **13380-89-7**, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-ol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (catalytic **deuteration** of carbonyl compds. or secondary alc.  
 compds. with heavy water in presence of palladium, platinum, rhodium,  
 ruthenium, or nickel)
- RN 13380-89-7 CAPLUS
- CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



- IT **13380-89-7DP**, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-ol, **deuterated**

725242-29-5DP, deuterated 725242-29-5P

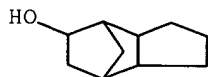
725242-30-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalytic **deuteration** of carbonyl compds. or secondary alc.compds. with heavy water in presence of palladium, platinum, rhodium,  
ruthenium, or nickel)

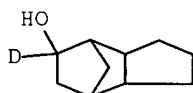
RN 13380-89-7 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



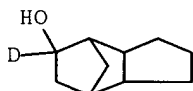
RN 725242-29-5 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-29-5 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-30-8 CAPLUS

CN 4,7-Methano-1H-inden-1,1,2,3,6,7,7-d7-5-ol, octahydro-2,3,3a,4,5,6,7,7a-d8-  
(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:199410 CAPLUS Full-text

DOCUMENT NUMBER: 112:199410

TITLE:  $\beta$ -Methyl- $\delta$ -valerolactone adductsINVENTOR(S): Kuroki, Masayuki; Yokoshima, Minoru; Maeda, Toshihiko;  
Yoshimura, Noriaki

PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan; Kuraray Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

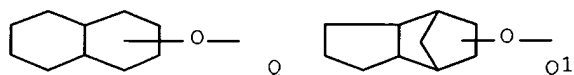
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

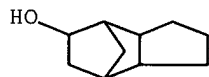
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01258645	A	19891016	JP 1988-83125	19880406
PRIORITY APPLN. INFO.: GI			JP 1988-83125	19880406



- AB R(COCH<sub>2</sub>CHMeCH<sub>2</sub>CH<sub>2</sub>O)nH [R = R<sub>1</sub>C<sub>6</sub>H<sub>4</sub>O(CH<sub>2</sub>CHR<sub>2</sub>O)<sub>m</sub>, CpH<sub>2</sub>p+10, perhydronaphthyloxy, perhydromethanoindanyloxy; R<sub>1</sub> = H, C<sub>1</sub>-12 alkyl; R<sub>2</sub> = H, Me; average m = 1-10; average n = 0.5-10; p = 1-20], whose (meth)acrylate esters are useful as diluents in UV-curable coatings, are prepared Thus, 374 parts poly(oxyethylene) p-nonylphenyl ether was treated with 684 parts β-methyl-δ-valerolactone at room temperature for 20 h to give 830 parts product with OH value 67.6.
- IC ICM C07C069-675
- CC 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 42
- IT 126161-91-9P 126161-92-0P **126161-93-1P** 126161-94-2P  
126286-45-1P 126286-48-4P 126305-36-0P  
RL: PREP (Preparation)  
(preparation of, as intermediate for methacrylate diluents, for UV-curable coatings)
- IT **126161-93-1P**  
RL: PREP (Preparation)  
(preparation of, as intermediate for methacrylate diluents, for UV-curable coatings)
- RN 126161-93-1 CAPLUS
- CN 2H-Pyran-2-one, tetrahydro-4-methyl-, homopolymer, octahydro-4,7-methano-1H-inden-5-yl ester (9CI) (CA INDEX NAME)
- CM 1
- CRN 13380-89-7
- CMF C10 H16 O

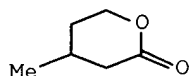


- CM 2
- CRN 97145-14-7

CMF (C6 H10 O2)x  
CCI PMS

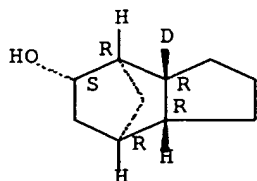
CM 3

CRN 1121-84-2  
CMF C6 H10 O2



L32 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1974:81650 CAPLUS Full-text  
 DOCUMENT NUMBER: 80:81650  
 ORIGINAL REFERENCE NO.: 80:13137a,13140a  
 TITLE: Dehydration of 5-hydroxytetrahydro-exo-dicyclopentadiene with acid  
 AUTHOR(S): Gates, Marshall; Zabriskie, John L., Jr.  
 CORPORATE SOURCE: Dep. Chem., Univ. Rochester, Rochester, NY, USA  
 SOURCE: Journal of Organic Chemistry (1974), 39(2), p 222-7  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB A study of the dehydration of 3a-**deuterio**-5-hydroxytetrahydro-exo-dicyclopentadiene (I) with acid suggests that the formation of 5,6-dihydro-exo-dicyclopentadiene (II) proceeds through 2,3-dihydro-exo-dicyclopentadiene (III) or the equilibrating ions formed from the latter by protonation followed by a 1,3-hydride shift, a 1,2-hydride shift, and proton loss.  
 CC 22-3 (Physical Organic Chemistry)  
 IT **42913-50-8**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydration of)  
 IT **10271-44-0**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydration of, mechanism of)  
 IT **42913-50-8**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydration of)  
 RN 42913-50-8 CAPLUS  
 CN 4,7-Methano-1H-inden-5-ol, octahydro-3a-d-, (3a $\alpha$ ,4 $\beta$ ,5 $\beta$ ,7.b  
 eta.,7a $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



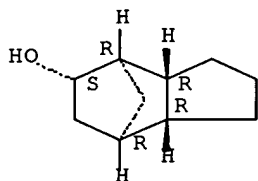
IT 10271-44-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydration of, mechanism of)

RN 10271-44-0 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro-, (3aR,4R,5S,7R,7aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



L32 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:32153 CAPLUS Full-text

DOCUMENT NUMBER: 74:32153

ORIGINAL REFERENCE NO.: 74:5169a,5172a

TITLE: Polymerization of  $\alpha$ -olefins

INVENTOR(S): Schmitt, Karl; Gude, Fritz; Samblebe, Reinhard

PATENT ASSIGNEE(S): Veba-Chemie A.-G.

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1918995	A	19701112	DE 1969-1918995	19690415
AT 301169	B	19720825	AT 1970-1008	19700204
GB 1304093	A	19730124	GB 1970-7318	19700216
BE 746667	A	19700731	BE 1970-746667	19700227
NL 7003130	A	19701019	NL 1970-3130	19700305
FR 2039082	A5	19710108	FR 1970-10329	19700323

PRIORITY APPLN. INFO.: DE 1969-1918995 A 19690415

AB Ti(OBu)<sub>4</sub>, Ti(OPr)<sub>4</sub>, titanyl acetylacetonate, or a similar Ti compound, is used with VO(OBu)<sub>3</sub>, V acetylacetonate, or a similar V compound and with Et<sub>2</sub>AlCl, EtAlCl<sub>2</sub>, Et<sub>2</sub>AlBr, iso-Pr<sub>2</sub>AlBr, or a similar Al compound, optionally containing Et<sub>3</sub>Al and ZnCl<sub>2</sub>, Et<sub>2</sub>Zn, Et<sub>2</sub>Cd, or a similar compound, to prepare polymerization catalysts for C<sub>2</sub>H<sub>4</sub>, propylene, 4-methyl-1-pentene, and similar  $\alpha$ -olefins. The catalysts have high catalytic activity, give colorless polymers even if the catalyst residue is not washed from the polymer, and give powdered polyolefins having good flow properties. Thus, 1 mole of a 1:3 molar mixture of Ti(OBu)<sub>4</sub> and VO(OBu)<sub>3</sub> in light petroleum was treated with 5.5 moles Et<sub>2</sub>AlCl to prepare a catalyst.

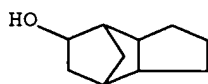
IC C08F001-42

CC 35 (Synthetic High Polymers)

IT 17501-79-0 19059-01-9 24742-16-3 28860-26-6 30860-71-0  
32673-47-5 32673-53-3, Malonic acid, titanium(4+) salt (2:1)

32673-54-4 **32719-33-8**RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for polyn. of olefins)IT **32719-33-8**RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for polyn. of olefins)

RN 32719-33-8 CAPLUS

CN 4,7-Methanoindan-5-ol, hexahydro-, titanium(4+) salt, exo- (8CI) (CA  
INDEX NAME)

● 1/4 Ti(IV)

L32 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1964:432551 CAPLUS Full-text

DOCUMENT NUMBER: 61:32551

ORIGINAL REFERENCE NO.: 61:5679e-h, 5680a-b

TITLE: Oxymercuration of endo- and exo-dicyclopentadienes

AUTHOR(S): Stille, J. K.; Stinson, S. C.

CORPORATE SOURCE: Univ. of Iowa, Iowa City

SOURCE: Tetrahedron (1964), 20(6), 1387-95

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 61:32551

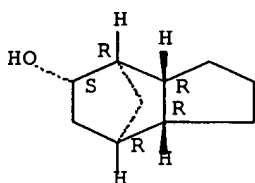
GI For diagram(s), see printed CA Issue.

AB cf. Traylor and Baker, CA 59, 10101g. To 2.2 g. LiAlH<sub>4</sub> in 15 ml. Et<sub>2</sub>O was added slowly 10.35 g. octahydro-exo-4,7-methanoinden-5-one in 20 ml. Et<sub>2</sub>O and the whole refluxed 1 hr. to give 6 g. octahydro-exo-4,7-methanoinden-endo-5-ol (I), b<sub>1.5</sub> 73°, n<sub>19.5D</sub> 1.5127. The procedure of Cristol (C., et al., CA 54, 20908e) with I gave 52% octahydro-endo-methoxy-exo-4,7-methanoindene, b<sub>9</sub> 81°, n<sub>19.5D</sub> 1.4860. Hydroboration of 2,3,3a,4,7,7a-hexahydro-endo-4,7-methanoindene gave octahydro-endo-4,7-methanoinden-exo-5-ol (II), m. 79.5-81° (MeNO<sub>2</sub>). II, as above, gave 47% octahydroexo-5-methoxy-endo-4,7-methanoindene (IIa), b<sub>6</sub> 84-6°, n<sub>19.5D</sub> 1.4923; CrO<sub>3</sub> oxidation of II in C<sub>5</sub>H<sub>5</sub>N gave the ketone, which was reduced with LiAlH<sub>4</sub> to give octahydro-endo-4,7-methanoinden-5-ol (III), m. 119.5-20° (petr. ether). III gave 52% octahydroendo-5-methoxy-4,7-methanoindene, b<sub>9</sub> 81°, n<sub>19.5D</sub> 1.4860. HgCl<sub>2</sub> and endo-dicyclopentadiene (IV) in MeOH gave 79% of the methoxymurcuric chloride adduct (V), m. 133°; the same reaction with exo-cyclopentadiene (Va) proceeded twice as rapidly to give 50% of the adduct (Vb), m. 135-7°. Hg(OAc)<sub>2</sub> (35 g.), 100 ml. H<sub>2</sub>O, and 10.7 g. IV shaken 10 hrs. gave 42% hydroxymurcuric acetate adduct (VI), m. 129-31° (CCl<sub>4</sub>); a similar reaction with V was faster and gave 42% unstable adduct (VIa), m. 130-5° (CCl<sub>4</sub>). To 40 g. V in 400 ml. H<sub>2</sub>O, with agitation, was added in small portions 152 g. 3% Na-Hg, the whole extracted with Et<sub>2</sub>O, and the Et<sub>2</sub>O extract dried and concentrated gave, via vapor phase chromatography a 1:1 mixture (VII) of IV and VIII; pure VIII (9.7 g.) was obtained by distillation, b<sub>7</sub> 77-8°, n<sub>20D</sub> 1.5007. Similarly, Vb gave 50% IX, b<sub>9</sub> 81-3°, n<sub>19.5D</sub> 1.4976. VI gave 33% X, b<sub>4</sub> 91°, m. 42-4° (MeNO<sub>2</sub>) (p-nitrobenzoate m. 121.5-2.5°), and VIa

gave 12.5% XI, b3-5 92°, n19.5D 1.5262 (p-nitrobenzoate m. 126.5-8.5°). VIII (5.65 g.), EtOH, and PtO2 gave 3.6 g. IIa. Similarly, 4.8 g. IX gave 3.2 g. octahydroexo-5-methoxy-exo-4,7- methanoindene (XII), b7 81, n20D 1.4855, 2.28 g. X gave 1.46 g. II, and 4.8 g. XI gave 1.58 g. octahydro-exo-4,7- methanoinden-exo-5-ol (XIII), m. 50.5-51°. V (20.4 g.), 200 ml. D2O, and 114 g. 3% Na-Hg gave 1.27 g. octahydro-exo-5-**deutero**-exo-6-methoxy-endo-4,7- methanoindene, b6 85-6°. The nuclear magnetic resonance spectra of some of these derivs. are discussed, the conclusion being that the mercuri group is cis or exo to the MeO or He groups.

- CC 39 (Organometallic and Organometalloidal Compounds)
- IT 77-80-5P, Tin, thiobis[triphenyl- 133-21-1P, 4,7-Methanoinden-5-ol, 3a,4,5,6,7,7a-hexahydro-(?), stereoisomers 338-48-7P, Germane, tributylfluoro 358-41-8P, Germane, triethylfluoro 994-28-5P, Germane, chlorotriethyl- 1067-10-3P, Germane, bromotriethyl- 1112-65-8P, Germane, acetoxytributyl 1441-22-1P, Tin, triphenyl(phenylthio)- 2117-36-4P, Germane, tributylchloro 2290-67-7P, Germane, triethylisothiocyano- 2587-86-2P, Germane, oxybis[tributyl 10271-44-0P, 4,7-Methanoindan-5-ol, hexahydro-, exo-exo- 13314-51-7P, Germane, triethyliodo- 22998-59-0P, Germane, dichlorodiisopropyl 24692-20-4P, Germanecarbonitrile, triethyl 53018-24-9P, 4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-5-methoxy-, stereoisomers 57831-55-7P, Germane, triethylisocyanato- 57879-96-6P, Tin, (methylthio)triphenyl- 79851-34-6P, Tin, (2-naphthylthio)triphenyl- 92168-27-9P, 4,7-Methanoinden-5-ol, 6-(acetoxymmercuri)-3a,4,5,6,7,7a-hexahydro-, stereoisomers 93818-38-3P, 4,7-Methanoinden-5-ol, 3a,4,5,6,7,7a-hexahydro-(?), p-nitrobenzoate, stereoisomers 94522-39-1P, 4,7-Methanoindene-6-d, 3a,4,5,6,7,7a-hexahydro-5-methoxy- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 108172-97-0P, Mercury, chloro(3a,4,5,6,7,7a-hexahydro-5-methoxy-4,7-methanoinden-6-yl)-, stereoisomers
- RL: PREP (Preparation)  
(preparation of)
- IT 10271-44-0P, 4,7-Methanoindan-5-ol, hexahydro-, exo-exo-  
RL: PREP (Preparation)  
(preparation of)
- RN 10271-44-0 CAPLUS
- CN 4,7-Methano-1H-inden-5-ol, octahydro-, (3aR,4R,5S,7R,7aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



L32 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1963:80843 CAPLUS Full-text  
 DOCUMENT NUMBER: 58:80843  
 ORIGINAL REFERENCE NO.: 58:13738e-h,13739a-d  
 TITLE: Bridged polycyclic compounds. XX. Cis stereochemistry



of the addition of methanol and water to  
endo-trimethylenenorbornene

AUTHOR(S): Cristol, Stanley J.; Gaston, Lyle K.; Johnson, Donald W.

CORPORATE SOURCE: Univ. of Colorado, Boulder

SOURCE: Tetrahedron Letters (1963) 185-9  
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

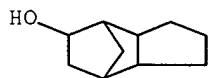
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

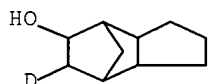
AB cf. CA 58, 10092d. H<sub>2</sub>SO<sub>4</sub> catalyzed addition of MeOH (or of H<sub>2</sub>O in MeOH) to the isomeric endo- and exo-tri-methylenenorbornenes (I, II) gave differing ratios of endo (III) and exo (IV) ring skeleton ethers (or alcs.); e.g., I and MeOH was reported to give 14.5: 85.5 III (R = OMe) (V)-IV (R = OMe) (VI), and II with MeOH to yield 3.5: 96.5 V-VI. It is shown now that reactions with I are entirely cis-exo addns. If the endo protonated  $\pi$  complex (VII) reacted directly with a solvent mol. by the equivalent of trans ring opening, the addition of MeOD and D<sub>2</sub>O to I would lead to the compds. (VIII, R = OMe, OD) (IX, X). I and II lead to III and IV in such amts. that at least 80% of III from I arises via a path different from that utilized in the addition to II. If the alternative path involved VII, then at least 80% of the III isomer isolated in the **deuterated** series would be labeled as in VIII, and this would be true if VII were formed and gave III by isomerization to a carbonium ion (XI). If, however, VII is not involved in the reaction sequence, III might be expected to be labeled as in XII, assuming exo protonation followed by transformation to carbonium ion intermediates, coordinating with solvent from the exo side. It seemed that VIII and XII could be distinguished by differences in nuclear magnetic resonance (n.m.r.) spectra. III (R = OH) (XIII) in CHCl<sub>3</sub> gave peaks at 6.07 (J 6.6 cycles/sec.), 7.6-9.2  $\tau$ . III (R = p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>) showed similar doublets at 5.46  $\tau$  (J 6.6 cycles/sec.) and 4.90  $\tau$  (J 6.6 cycles/sec.). It appeared that the principal coupling was due to interaction between H and the C-3 H eclipsed with it, and that this coupling would be observed in XII, but would not appear in VIII. Treatment of 5,6-endo-trimethylene-2,3-exo-epoxynorbornane with LiAlD<sub>4</sub> gave VIII (R = OH), showing a broad singlet at 6.02  $\tau$ ; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub> derivative m. 123-6°, n.m.r. singlet at 4.89  $\tau$ . Addition of B<sub>2</sub>D<sub>6</sub> to I followed by oxidation gave XII (R = OH), n.m.r. doublet at 6.09  $\tau$  (J 6.9 cycles/sec.); p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub> derivative m. 128-9°, doublet at 4.99  $\tau$  (J 7.0 cycles/sec.). I (8.04 g. containing 9.7% II and 1.5% dicyclopentadiene), 5.5 ml. D<sub>2</sub>SO<sub>4</sub>, 2.2 ml. D<sub>2</sub>O, and 46 ml. MeOD refluxed 10 hrs. with stirring and treated with 10 g. Na<sub>2</sub>SO<sub>4</sub>, poured into H<sub>2</sub>O, and extracted with Et<sub>2</sub>O, the Et<sub>2</sub>O evaporated, and the residue [5.2% I, 10.3% V, 68.7% VI, 2.6% XIII, and 13.2% IV (R = OH) (XIV) by gas phase chromatography] chromatographed on Al<sub>2</sub>O<sub>3</sub>, eluted with pentane, and the ether mixture separated on a 2 m. (3/8 in.) 30% Carbowax 1540-Chromosorb column at 123° in 88 ml./min. gave I, XIV, and V in 26, 106, and 136 min. V showed a fairly sharp doublet at 6.74.  $\tau$  (J.6.7) and the spectrum indicated that less than 10% of IX could be present as a contaminant in the XIII (R = OMe) produced. Further elution with Et<sub>2</sub>O gave the alc. fractions which were converted to p-nitrobenzoates inseparable into isomers. The esters reduced with LiAlH<sub>4</sub>, chromatographed on Al<sub>2</sub>O<sub>3</sub>, and separated by gas chromatography on a 1 m. (1/4 in.) 30% Carbowax 1540 column at 130° with 88 ml. He/min. gave XIV and XIII in 66 and 86 min., resp. XIII showed a doublet at 6.08  $\tau$  (J 6.6 cycles/sec.). Less than 10% of X could be present in the XII (R = OH) produced. Clearly cis-exo addition of both the H and R portions of the addenda occurs and the endo-protonated complex VII is excluded as a significant intermediate in the addition reaction to I leading to III. It is suggested that at least one of the intermediates involved is a classical ion

such as XI, or that a cis addition 4-center transition state is involved, in which no carbonium ion is developed.

CC 32 (Physical Organic Chemistry)  
 IT 2198-08-5 2415-40-9 2628-89-9 **13380-89-7** 19398-83-5  
 68628-62-6 **96655-49-1** 97811-11-5  
 (Derived from data in the 7th Collective Formula Index (1962-1966))  
 IT **13380-89-7 96655-49-1**  
 (Derived from data in the 7th Collective Formula Index (1962-1966))  
 RN 13380-89-7 CAPLUS  
 CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



RN 96655-49-1 CAPLUS  
 CN 4,7-Methanoindan-6-d-5-ol, hexahydro- (7CI) (CA INDEX NAME)



=> d his nofil

(FILE 'HOME' ENTERED AT 15:58:41 ON 15 JAN 2008)

FILE 'CAPLUS' ENTERED AT 15:58:51 ON 15 JAN 2008  
 E US2005-539188/APPS

L1 1 SEA ABB=ON PLU=ON US2005-539188/AP  
 SEL RN  
 D SCA  
 E DEUTERATION/CT  
 E E3+ALL  
 L2 2077 SEA ABB=ON PLU=ON DEUTERATION+PFT/CT  
 E DEUTERATION CATALYSTS+ALL/CT  
 L3 287 SEA ABB=ON PLU=ON DEUTERATION CATALYSTS+PFT,NT/CT  
 L4 2148 SEA ABB=ON PLU=ON L2 OR L3

FILE 'REGISTRY' ENTERED AT 16:00:21 ON 15 JAN 2008

FILE 'CAPLUS' ENTERED AT 16:00:34 ON 15 JAN 2008

L5 TRA PLU=ON L4 1- RN : 22168 TERMS

FILE 'REGISTRY' ENTERED AT 16:01:30 ON 15 JAN 2008

L6 22168 SEA ABB=ON PLU=ON L5  
 L7 952 SEA ABB=ON PLU=ON L6 AND (PD OR PT OR RH OR RU OR NI OR CO)/ELS

FILE 'CAPLUS' ENTERED AT 16:03:17 ON 15 JAN 2008

L8 154222 SEA ABB=ON PLU=ON L7(L)CAT+NT/RL  
L9 247 SEA ABB=ON PLU=ON L8 AND L4  
L10 115 SEA ABB=ON PLU=ON L2 AND L3 AND L8

FILE 'REGISTRY' ENTERED AT 16:04:58 ON 15 JAN 2008  
L11 STR

FILE 'CAPLUS' ENTERED AT 16:10:55 ON 15 JAN 2008  
S L11

FILE 'REGISTRY' ENTERED AT 16:11:21 ON 15 JAN 2008  
L12 50 SEA SUB=L6 SSS SAM L11

FILE 'CAPLUS' ENTERED AT 16:11:21 ON 15 JAN 2008  
L13 68 SEA ABB=ON PLU=ON L12

FILE 'REGISTRY' ENTERED AT 16:11:26 ON 15 JAN 2008  
L14 50 SEA SUB=L6 SSS SAM L11  
L15 2492 SEA SUB=L6 SSS FUL L11  
L16 1209 SEA ABB=ON PLU=ON L15 AND D/ELS

FILE 'CAPLUS' ENTERED AT 16:12:27 ON 15 JAN 2008  
L17 897 SEA ABB=ON PLU=ON L16(L)PREP+NT/RL  
L18 40 SEA ABB=ON PLU=ON L17 AND L9  
L19 22 SEA ABB=ON PLU=ON L17 AND L10  
L20 1 SEA ABB=ON PLU=ON L1 AND L1

FILE 'CAPLUS' ENTERED AT 16:13:16 ON 15 JAN 2008  
D QUE L19  
D L19 IBIB ABS HITIND HITSTR TOT  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 16:15:20 ON 15 JAN 2008  
L21 49 SEA ABB=ON PLU=ON (7440-16-6/BI OR 108-93-0/BI OR 13380-89-7/  
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7440-06-4/BI OR 7440-18-8/BI OR 79-31-2/BI OR 106-35-4/BI OR  
108-94-1/BI OR 110-43-0/BI OR 123-19-3/BI OR 127-09-3/BI OR  
13380-94-4/BI OR 14044-94-1/BI OR 18153-61-2/BI OR 21273-02-9/B  
I OR 3385-61-3/BI OR 350820-09-6/BI OR 497-38-1/BI OR 51209-49-  
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OR 67-64-1/BI OR 725242-18-2/BI OR 725242-19-3/BI OR 725242-21-  
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7440-02-0/BI OR 7440-48-4/BI OR 7789-20-0/BI OR 78-93-3/BI OR  
79-41-4/BI OR 91468-78-9/BI)  
L22 10 SEA ABB=ON PLU=ON L21 AND NR>2  
D SCA  
L23 2 SEA ABB=ON PLU=ON L22 AND ?DECAN?/CNS  
D SCA  
L24 1 SEA ABB=ON PLU=ON L23 AND C10H16O/MF  
D  
SEL RN  
L25 3 SEA ABB=ON PLU=ON 13380-89-7/CRN  
D SCA

FILE 'CAPLUS' ENTERED AT 16:17:52 ON 15 JAN 2008  
L26 2 SEA ABB=ON PLU=ON L25  
D QUE L26

D L26 IBIB ABS HITSTR TOT

FILE 'REGISTRY' ENTERED AT 16:18:52 ON 15 JAN 2008

L27 STR 13380-89-7

L28 52 SEA FAM FUL L27

FILE 'CAPLUS' ENTERED AT 16:19:11 ON 15 JAN 2008

L29 133 SEA ABB=ON PLU=ON L28

L30 168165 SEA ABB=ON PLU=ON ?DEUTER?

L31 4 SEA ABB=ON PLU=ON L29 AND L30

L32 6 SEA ABB=ON PLU=ON L31 OR L26

FILE 'CAPLUS' ENTERED AT 16:19:51 ON 15 JAN 2008

D QUE L32

D L32 IBIB ABS HITIND HITSTR TOT